PB86-209095

Coal Gasification Environmental Data Summary: Organics

Radian Corp., Austin, TX

Prepared for

Environmental Protection Agency
Research Triangle Park, NC

Apr 86

U.S. Department of Commerce
National Technical Information Service
NTIS

PB86-209095

EPA/600/7-86/015d
April 1986

COAL GASIFICATION ENVIRONMENTAL DATA SUMMARY:
ORGANICS

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EPA Contract No. 68-02-3137

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SPRINGFIELD, VA. 22161

TECHNICAL REPORT DATA

(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA/600/7-86/015d	2.	3. RECIPIENT'S ACCESSION NO. PB86-209095/AS
4. TITLE AND SUBTITLE Coal Gasification Environmental Data Summary: Organics		5. REPORT DATE April 1986
		6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) Karl J. Bombaugh		8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS Radian Corporation P.O. Box 9948 Austin, Texas 78766		10. PROGRAM ELEMENT NO.
		11. CONTRACT/GRANT NO. 68-02-3137
12. SPONSORING AGENCY NAME AND ADDRESS EPA, Office of Research and Development Air and Energy Engineering Research Laboratory Research Triangle Park, NC 27711		13. TYPE OF REPORT AND PERIOD COVERED Final; 9/84 - 12/85
		14. SPONSORING AGENCY CODE EPA/600/13

15. SUPPLEMENTARY NOTES AEERL project officer is William J. Rhodes, Mail Drop 62B, 919/541-2853.

16. ABSTRACT The report summarizes the organics data from environmental assessments of several low- and medium-Btu coal gasification processes conducted between 1977 and 1981 under the sponsorship of the U.S. EPA. This data summary focuses on the concentration, composition, and mass flow of organics in the major streams of the various gasifier-related processes. Many compounds in the organics from the major gaseous-, aqueous, and solid-phase streams of the processes are identified. Organic compositions and stream concentrations among plants and plant streams are compared.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Pollution	Pollution Control	13B
Coal Gasification	Stationary Sources	13H
Coal	Environmental Assessment	21D
Organic Compounds		07C
Assessments		14B
Chemical Analyses		07D

18. DISTRIBUTION STATEMENT Release to Public	19. SECURITY CLASS *(This Report)* Unclassified	21. NO. OF PAGES 181
	20. SECURITY CLASS *(This page)* Unclassified	22. PRICE $16.95

NOTICE

This document has been reviewed in accordance with U.S. Environmental Protection Agency policy and approved for publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

ABSTRACT

This report contains a summary of the organics data from Environmental Assessments of several low- and medium-BTU coal gasification processes conducted between 1977 and 1981 under the sponsorship of the U. S. Environmental Protection Agency. The focus of this data summary is on the concentration, composition, and mass flow of organics in the major streams of the various gasifier-related processes. Numerous compounds in the organics from the major gaseous-, aqueous-, and solid-phase streams of the several processes are identified. Organic compositions and stream concentrations among plants and plants' streams are compared.

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ACKNOWLEDGMENTS

The helpful suggestions of Project Director, R. A. Magee, and of the reviewers, M. P. Kilpatrick and R. G. Wetherold, are gratefully acknowledged. Also, Section 3, Process Descriptions, was prepared by F. D. Skinner, the literature search was provided by N. P. Meserole, and editorial support was provided by A. E. Behl.

SECTION 1

INTRODUCTION

This report, prepared for the Air and Energy Engineering Research Laboratory of the U.S. Environmental Protection Agency, provides a collection and reduction of data that pertains to the organics in coal gasification process and discharge streams. During the past decade, EPA/AEERL has conducted source test and evaluation programs at commercial-, pilot-, and bench-scale coal gasification facilities. The objectives of these programs were to provide test data for:

- characterizing regulated and nonregulated species in process waste streams;
- evaluating pollution control process performance;
- developing sampling and analytical methods for characterizing constituents in process and waste streams;
- evaluating the potential health and ecological effects of process waste streams;
- developing pollution control schemes for treating gaseous, liquid, and solid waste streams;
- providing input to federal, state, and local regulatory agencies; and
- providing input to health studies.

These programs were conducted on several types of gasifiers using different coal feedstocks (Table 1). The facilities were selected based on the greater availability of process, gas, liquid, and solid phase data. Results of these investigations are documented in a number of government reports, symposia proceedings, and journal publications (1 thru 17). The tests varied in scope as well as in breadth and dealt with a range of pollutant groups (e.g., trace metals, organics, sulfur species, nitrogen species, and hydrocarbons). Some studies dealt primarily with wastewater; others investigated all types of streams: gaseous, organic-liquid, and aqueous- and solid-waste. The data from several of these test sites are distributed over more than one document so that several documents must be consulted to obtain comprehensive pictures of any pollutant-concern relating to more than one gasifier.

It is therefore the objective of this report to present a compilation of currently available data that relate specifically to the organics levels in the various streams of the several types of coal gasifiers that were investigated under this program. In addition to presenting a coherent compilation and summary, these data have been consolidated in an effort to enable an interpretative evaluation of:

- trends or correlations of organics behavior across processes,
- trends or correlations in the context of control approaches,
- specific characteristics of individual processes, and
- recommendations for monitoring commercial-scale systems to further define environmental issues or apparent trends in pollutant behavior.

This data consolidation and evaluation should make it possible to:

- recognize process-specific characteristics for both synfuels production and pollution control technologies which should influence the

TABLE 1. SOURCE TEST AND EVALUATION PROGRAM

Plant	Gasification Process	Fuel
Fort Snelling	Wellman-Galusha (low BTU)	N. Dakota Lignite
Glen-Gery	Wellman-Galusha (low BTU)	Anthracite
Holston	Willputte/Chapman (low BTU)	Bituminous Coal
Kosovo	Pressurized, fixed-bed gasifier	Lignite
Modderfontein	Koppers-Totzek entrained-bed	High Volatile Bituminous Coal
Ptolemais	Koppers-Totzek entrained-bed	Bituminous Coal
Worcester	Riley Gas Producer (low BTU gasifier)	Lignite
Oberhausen-Holten	Texaco entrained-bed	Illinois No. 6 Bituminous Coal
Duluth, University of Minnesota	Foster-Wheeler/STOIC (low BTU gasifier)	Lignite
Madison, PA	Kellogg-Rust/Westinghouse, fluidized-bed process development unit	WY Subbituminous Pittsburgh #8 Bituminous ND Lignite
	Other Programs	
Homer City	Bi-Gas Pilot Plant	Pittsburgh #8 Bituminous Coal
SASOL 1	Lurgi Mark IV (modified)	Ky #9 Bituminous Coal

areas of emphasis and scope of future monitoring activities including monitoring for Synthetic Fuels Corporation (SFC)-supported facilities, and

- define data interpretation and presentation approaches which will aid the evaluation of the data addressing particular areas of concern in mitigating environmental and health problems with existing and future facilities.

In this report the term "organics" refers to any compound, or group of components, that contain both carbon and hydrogen. Compounds containing other elements such as oxygen, nitrogen, and sulfur in addition to carbon and hydrogen are also considered to be organic. Methane, however, is excluded from the group since in this technology it is more appropriately considered with the fixed gases.

This report presents the data in a unified format so that comparisons between processes can be made. In doing so, compromises had to be made with the data to achieve a unified base for comparison. The problem of presenting the organic data in a unified format was exacerbated by the complexity of the organic mixtures; the complexity of the various species; and the nature of analyses that, in some instances, were able to find certain species only when sought. As a result, some species measured in the organics from one process may not be listed in the organics from a similar process only because they were not sought specifically; and they were not sought because such speciation was not within the initially defined objectives of that specific source test. As the analytical protocol evolved, complexity and specificity increased concurrently so that compounds found in later tests may have been present but not sought in process streams that were tested earlier. A specific effort has been made to differentiate between the designation "ND", not detected, (meaning looked for and not found) and "NA" (meaning not analyzed). It must be emphasized that a "not analyzed" classification does not mean that a compound is either present or not present, only that it was not analyzed. In addition, many compounds that have not been identified, and therefore are not listed, may be present in these complex organic mixtures. The data presented here should not be construed as being either complete or comprehensive.

Several types of organic data were generated by these source tests:

- bulk organic loading based on AEERL's protocol for a Level 1 environmental assessment:
    - Total chromatographable organics (TCO) hereafter referred to as volatile organics (VO),
    - Gravimetrically determined organics (GRAV) hereafter referred to as nonvolatile organics (NVO), and
    - Liquid chromatographic (LC) fractions (seven) separated according to compound polarity;
- light hydrocarbons in gas streams as determined by gas chromatography (GC) or GC-mass spectrometric (GC-MS) analyses;
- water quality parameters pertaining to organic content of aqueous streams and leachates (e.g., total organic carbon);
- detailed speciation based on GC-MS analyses; and
- "fingerprints" as provided by GC and infrared spectrophotometry (IR).

Major emphasis has been placed on the first and fourth categories, bulk organics and speciation by GC-MS, in identifying stream pollutants; however, all five categories provide useful information for comparing processes.

The many coal gasification processes can generally fit into two categories, tar-producing (fixed-bed) and tar-free (fluid- and entrained-bed). Since little information is available about the very limited organics in the streams from tar-free processes, this report deals primarily with the organics from tar-producing processes.

Following this introduction, Section 2 presents summary statements and conclusions. Section 3 presents a description of the several gasification processes tested. Section 4 provides a description of test methodologies used to obtain the organics data. Emphasis in Section 4 is on the principle of the method rather than on the detailed procedures used for each test. Section 5 presents the results, beginning with a data summary, followed by subsections containing the tabulations of detailed analyses data from each process and concludes with a comparison of the qualitative profiles of organics from several streams using techniques that are selective to specific compositional characteristics.

SECTION 2

CONCLUSIONS

The conclusions drawn from this evaluation point out the similarities and dissimilarities in the gasification processes reviewed. The major similarities in the data are:

- the tar-producing gasifiers, operated on coal with similar volatiles content, produced approximately 30 Kg of condensable organics in the product gases per metric ton of feed coal;
- these organics generally were similar in composition; and
- no gasifier showed a trend toward the production of any specific class of compounds or species (hazardous or non-hazardous) that was significantly different from the others.

The data indicate that the five tar-producing gasifiers (Chapman, Wellman-Galusha [Fort Snelling], Riley, Foster-Wheeler/STOIC, and the Lurgi-type [Kosovo]) produce similar amounts of similar kinds of organics. However, these data are dependent upon the analytical techniques employed. Hundreds of components were detected, many species were identified, and many identifications were made at the component class or subclass level (e.g., alkyl benzenes). The total identification of these components was far from complete as would be expected from the survey nature of these studies. The non-polar organics identified were primarily paraffins (including long straight chain paraffins), aromatics (benzenes, alkyl benzenes, naphthalenes, and alkyl naphthalenes), and polycyclic aromatics (including alkyl polycyclic aromatics and polycyclic hydro-aromatics). The polar organics consisted of hydroxyaromatics (phenols and alkyl phenols), aromatic amines, and nitrogen heterocyclics. The organics contained lesser amounts of heterocyclic compounds containing oxygen, sulfur, and multi-heterocyclic compounds (e.g., thiazoles).

Detailed analyses tended to be pre-directed to known components of concern such as priority pollutants or selected polynuclear aromatics and were generally limited to single column gas chromatography-mass spectrometry without additional separation and confirmation. Speciation was not consistent across the data base, and no valid comparison of species distribution across the gasifiers as a group can be made. This limitation is made more severe in several cases because the mass of an extensive list of identified compounds represented less than ten percent of the total organic mass in a stream. For the Chapman gasifier, however, relatively few components comprised the major portion of the speciated mass. Overall, the speciations do not provide a complete statement of composition for the organics arising from the gasification process, but they do identify and quantify many species considered to be environmentally significant. Additional compounds of equal or greater significance also may have been present. The gasifiers surveyed displayed some dissimilarities which, in general, were substantiations of the overall behavior of organics in gasification processes.

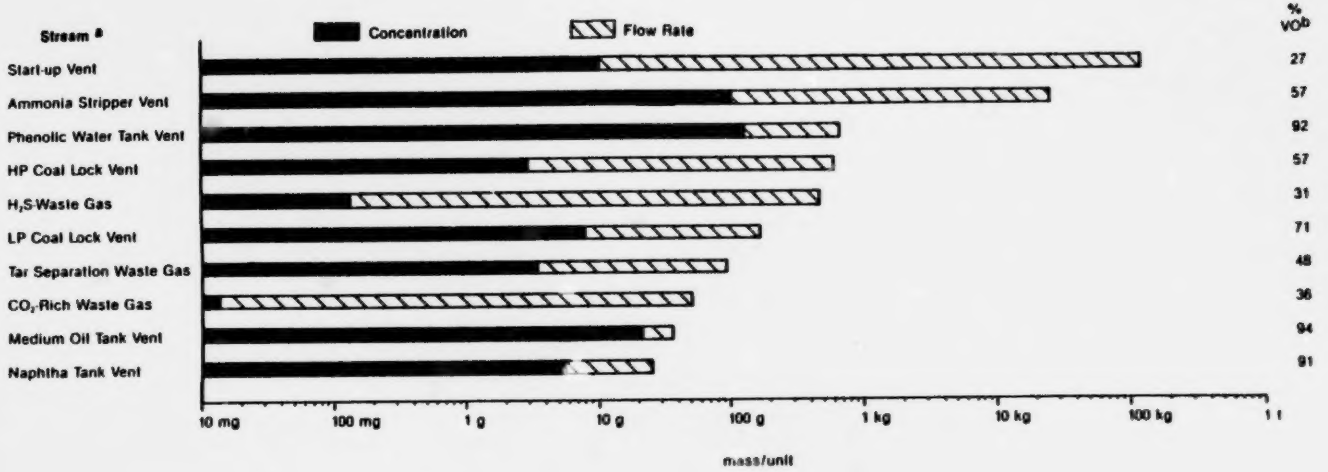
The organics in the crude product gas result largely from thermal devolatilization of coal. Therefore, it is not surprising that the product gas from the Wellman-Galusha gasifier (Glen-Gery), operated on anthracite, contained virtually no condensable organics. The bottom gas from the Foster-Wheeler/STOIC gasifier which is produced from the coked coal was also practically organic-free. The entrained-bed processes (Texaco, KRW and Koppers-Totzek) force the devolatilized material to pass through the gasification zone so their product gases were also much lower in condensable organics. Trace amounts of phenol were found in the aqueous streams from these processes. It is also noteworthy that the organic loadings of the ash from the tar-producing gasifiers were all between 300 and 600 ppm except for the Foster-Wheeler/STOIC which was only 1 ppm.

Organics in crude product gas can impact the environment either by escaping from the process through a discharge stream or a leak or by increasing the level of pollutants in combustion flue gas. Several conclusions concerning the environmental significance of organics in product gas can be made from the collected data:

- The impact of organics escaping to the environment is a process-specific and a stream-specific problem because the composition of the organics mixture is influenced by temperature and by contact with both aqueous and organic solvents. For example, at the Chapman site the organics discharged from the stripper vent (45% VO) were different from the organics trapped from either the crude gas (16% VO) or the tar (5.0% VO).

- When selective treatments are employed, such as at Kosovo where a combination of aqueous scrubbing, selective gas cleaning (Rectisol), and selective water cleaning (Phenosolvan) are used, the organic composition is altered considerably. Lipophilic components were enriched in the naphtha and medium oil while the hydrophilic components were concentrated in the water and accumulated in the crude phenol. Both types of components were concentrated, to some extent, by the thermally condensed tar. In such a system, the composition of the condensable or extractable organic is stream specific.

A survey of organic mass loadings, as in Figure 1, indicates the potential for pollution from that source, but it does not describe the composition nor define the risk potential. LC fractionation as used in this study can indicate whether the bulk of the organics is primarily polar or non-polar but more detailed analyses are required to assess the severity of pollution or the potential for environmental effects. Nevertheless the organic composition and mass loading data assembled here provide valuable information for use in environmental control technology.



[a] Not shown - Tar tank vent - Discharging 8 g/hr at a flow rate of 0.55 m^3/hr.

[b] VO = Volatile organics.

[c] The scale for concentration is mass/m^3 measured from the ordinate, and the scale for mass flow rate is mass/hr. The volumetric flow rate is m^3/hr measured from unity. For example, the ammonia stripper vent concentration is about 100 g/m^3, the mass flow rate is 24 kg/hr, and the volumetric flow rate is 240 m^3/hr.

Figure 1. Key Kosovo gaseous streams, in order of decreasing mass flow of condensable organics.

SECTION 3

PROCESS DESCRIPTIONS

INTRODUCTION

This section presents brief descriptions and comparisons of the coal gasification facilities for which data are presented in this report. The following types of gasifiers and facilities are included:

- Chapman low-Btu industrial gasifiers at Kingsport, Tennessee;
- Wellman-Galusha low-Btu gasifiers at the Bureau of Mines Twin Cities Metallurgy Research Center, Fort Snelling, Minnesota, and Glen-Gery Brick Company, York, Pennsylvania;
- Riley Gas Producer low-Btu gasifier at Worcester, Massachusetts;
- Foster-Wheeler/STOIC low-Btu industrial gasifier at the University of Minnesota, Duluth (UMD);
- Lurgi-type medium-Btu commercial gasifiers at Kosovo, Yugoslavia;
- Kellogg-Rust/Westinghouse (KRW) medium-Btu gasifier PDU at Madison, Pennsylvania;
- Koppers-Totzek medium-Btu commercial gasifiers at Modderfontein, South Africa;

- Koppers-Totzek (GKT) medium-Btu commercial gasifier at Ptolemais, Greece; and

- Texaco medium-Btu demonstration gasifier at the Ruhrkohle/Ruhrchemie facility in Oberhausen-Holten, Federal Republic of Germany.

Table 2 presents a summary of the features of the coal handling/preparation, coal feeding, gasification, and downstream processes (including gas cleanup and ash removal/handling) present at each facility. The similarities and differences will be discussed in more detail later; however, some of the salient differences between processes are summarized below:

- Oxygen versus Air-Injection: Gasifiers that use air as their source of oxygen produce a gas having a lower calorific value than those that use pure or nearly pure oxygen. This is due to the nitrogen diluent present in air. Chapman, Wellman-Galusha, Riley, and Foster-Wheeler/STOIC gasifiers are of the so-called "low-Btu" type, while the Koppers-Totzek and Texaco gasifiers both produce "medium-Btu" gas. The Lurgi and KRW gasifiers can be operated in either mode; the data presented here were obtained on systems producing medium-Btu gas.

- Bed Type: There are three principal gasifier bed types: moving-bed, fluidized-bed, and entrained-bed. Moving-bed (sometimes referred to as fixed-bed) gasifiers feature a layer of coal which is generally supported on a grate through which air (or oxygen) and steam are passed. In thin bed systems, less than a 0.5 m layer of coal is maintained on the coal grate. In thick bed systems, bed depths of 2 to 5 m are more typical. The direction of movement of the coal relative to the gas is countercurrent. In fluidized-bed gasifiers the upward velocity of the gas stream is such that the fluid drag forces nearly balance the downward forces due to the weight of the coal/ char particles. The particles act as if they were a turbulent fluid. In entrained-bed gasifiers,

TABLE 2. COMPARISON OF COAL GASIFICATION FACILITIES

	Chapman	Wellman-Galusha (Fort Snelling)	Wellman-Galusha (Glen-Gery)	Riley	Foster-Wheeler/STOIC
COAL HANDLING					
Receive presized coal	X	X	X	X	X
Crush/pulverize					
Screen		X			X
Thermal drying					
Slurrying					
Air classifying					
COAL FEEDING					
Lock hoppers		X	X	X	X
Screw feed/entrainment					
Slurry pumping					
Barrel valve	X				
GASIFICATION					
Atmospheric (A)/Pressurized (P)	A	A	A	A	A
Moving- (M)/Fluid- (F)/Entrained-bed (E)	M	M	M	M	M
Thin bed (T)/Deep bed (D)	T	D	D	T	D
Slagging (S)/Agglomerating (A)/Dry ash (D)	D	D	D	D	D
Single-stage (S)/Two-stage (T)	S	S	S	S	T
Cocurrent (C)/Countercurrent (CC)	CC	CC	CC	CC	CC
Air blown (A)/O_2 blown (O)	A	A	A	A	A
GAS CLEANUP					
Cyclones	X	X	X	X	X
ESP					X
Quench/Scrubbing	X				
Acid gas removal					
ASH REMOVAL/HANDLING					
Lockhoppers					
Ash plow	X			X	X
Slide valve		X	X		
Water quench	X	X	X	X	X
Conveyor/Drag chain	X				X

(continued)

TABLE 2. COMPARISON OF COAL GASIFICATION FACILITIES (Continued)

	Lurgi-type (Kosovo)	KRW PDU	Koppers-Totzek (Modderfontein)	Koppers-Totzek (Ptolemais)	Texaco (Ruhrchemie)
COAL HANDLING					
Receive presized coal					
Crush/pulverize	X	X	X	X	X
Screen	X				
Thermal drying	X	X	X	X	
Slurrying					X
Air classifying		X			
COAL FEEDING					
Lock hoppers	X	X			
Screw feed/entrainment			X	X	
Slurry pumping					X
Barrel valve					
GASIFICATION					
Atmospheric (A)/Pressurized (P)	P	P	A	A	P
Moving- (M)/Fluid- (F)/Entrained-bed (E)	M	F	E	E	E
Thin bed (T)/Deep bed (D)	D	D	—[a]	—[a]	—[a]
Slagging (S)/Agglomerating (A)/Dry ash (D)	D	A	S	S	S
Single-stage (S)/Two-stage (T)	S	S	S	S	S
Cocurrent (C)/Countercurrent (CC)	CC	CC	C	C	C
Air blown (A)/O_2 blown (O)	O	O	O	O	O
GAS CLEANUP					
Cyclones		X			
ESP			X	X	
Quench/Scrubbing	X	X	X	X	X
Acid gas removal	X		X	X	X
ASH REMOVAL/HANDLING					
Lockhoppers	X	X			X
Ash plow					
Slide valve					
Water quench	X		X	X	X
Conveyor/Drag chain	X		X	X	X

[a] Not applicable.

the coal and gases move in the same direction (co-current). Of the gasifiers represented here, only the KRW is a fluidized-bed gasifier; entrained-bed gasifiers include the Koppers-Totzek and Texaco gasifiers. All the rest are of the fixed-bed type.

- Single-stage versus Two-stage: In single-stage gasifiers, the raw product gas is taken off at a single location. In two-stage gasifiers, two separate raw product gas streams are generated. In a fixed-bed, two-stage design the upper gas product is richer in heavier hydrocarbon gases and aerosols formed by the release of coal volatile matter and water vapor resulting from the release of moisture in the feed coal. The lower gas product is richer in lighter combustible gases such as carbon monoxide and hydrogen. The only two-stage gasifier presented here is the Foster-Wheeler/STOIC gasifier.

- Atmosphere Pressure versus Elevated Pressure: Operation at elevated pressure allows the use of smaller vessels for equivalent gas production. Increased partial pressures of reactive gases may increase reaction rates and/or alter reaction equilibria in both the gasifier and in downstream units. Additional effects of pressurized operation include:

--reduced needs for compression of raw gas prior to downstream treatment units (e.g., physical absorption type acid gas removal processes) or prior to injection into a pipeline transmission system.

--generation of flash gases from depressurization of by-product liquids, resulting in an additional waste gas stream.

Of the gasifiers considered here, only three were operated at elevated pressure; the Lurgi-type (Kosovo), KRW, and Texaco

(Ruhrkohle/Ruhrchemie) gasifiers. The rest were operated at or near atmospheric pressure.

The remainder of this process description section consists of two subsections: the first discusses and compares the gasification processes (including coal preparation and coal feeding), while the second deals with downstream processing operations.

SUMMARY AND COMPARISON OF GASIFICATION OPERATIONS

Coal gasification involves the conversion of coal to gaseous species which can be burned as fuels or which can be used as feedstocks in the formation of fuels or other products. There are several general types of phenomena which occur during coal gasification which are common to all processes. These include coal drying and devolatilization, gasification, oxidation (or combustion), water-gas shift, volatilization and reaction of coal sulfur and nitrogen, and production of unreacted residuals (ash). Each of these may occur in different areas of the gasification reactor depending on the method used to contact the coal and the reactant gases.

Drying and Devolatilization

As the coal is heated, moisture is given off and the volatile fraction undergoes pyrolysis (i.e., thermal decomposition). The composition of the volatiles (some of which may be liquids or even solids at ambient conditions) depends on a number of factors including coal rank, coal particle thermal history (e.g., heating rate, duration of heating, and final temperature reached), and the composition and pressure of the reactant gas. Anthracite, for example, gives off relatively little volatile matter compared with bituminous coal or lignite. If devolatilization occurs at relatively low temperatures, the volatile fraction contains appreciable amounts of tar and oil aerosols. If devolatilization occurs at higher temperatures, these tars and oils are largely converted, by further pyrolysis into lighter hydrocarbons, methane, hydrogen, carbon monoxide, and carbon dioxide.

Gasification

In the gasification zone, various reactions occur between the carbon in the coal and the hot gases present in the oxidation zone. The principal gasification reactions of interest are:

$$C + CO_2 + \text{heat} \longrightarrow 2CO$$

$$C + H_2O + \text{heat} \longrightarrow CO + H_2$$

$$C + 2H_2 \longrightarrow CH_4 + \text{heat}$$

As can be seen, the primary products of gasification are carbon monoxide, hydrogen, and methane. The energy required by the first two reactions is furnished by the sensible heat of the gases leaving the oxidation zone. The extent to which these competing reactions proceed to completion depends on factors such as pressure, temperature, residence time, and reactant concentrations.

Oxidation (Combustion)

Oxidation involves the heterogeneous reaction between coal carbon and oxygen to produce CO and CO_2:

$$C + O_2 \longrightarrow CO_2 + \text{heat}$$

$$C + 1/2\ O_2 \longrightarrow CO + \text{heat}$$

These reactions result in the release of energy that allows the gasification reactions to proceed. The ratio of carbon monoxide to carbon dioxide formed in the oxidation zone depends on the oxygen partial pressure and the temperature. If excess oxygen is present, some of the carbon monoxide will be converted to CO_2 by gas phase oxidation.

In addition, in entrained-bed gasifiers and some fluidized-bed gasifiers where devolatilization occurs in an oxygen-rich environment, tars and oils and other organics are also oxidized in the gas phase, forming carbon monoxide, carbon dioxide, and hydrogen.

Water-Gas Shift

An important gas-phase reaction occurring in the gasifier involves the equilibrium among carbon monoxide, carbon dioxide, hydrogen, and water vapor:

$$CO + H_2O \rightleftharpoons CO_2 + H_2$$

The composition of the raw product leaving the gasifier is significantly influenced by this equilibrium. High temperature favors the formation of carbon monoxide and water vapor. The relative partial pressures of the various reactants also influence the equilibrium composition.

Sulfur and Nitrogen Reactions

Coal contains varying amounts of sulfur and nitrogen. Significant reaction products formed from these elements during gasification include ammonia, hydrogen cyanide, hydrogen sulfide, carbonyl sulfide, and other organic sulfur species (such as mercaptans). The quantities of such species formed depend on a number of factors including coal sulfur and nitrogen content, temperature, pressure, and hydrogen concentration in the gas. The ratio of carbonyl sulfide to hydrogen sulfide is a particularly important concern because this ratio can affect the selection, design, and performance of downstream acid gas removal and sulfur recovery processes. As with the water-gas shift reactions discussed above, the ratio of COS to H_2S in the raw gas is affected by the steam and carbon dioxide content of the gas due to the chemical equilibrium which is maintained at high temperatures among these four species:

$$H_2S + CO_2 \rightleftharpoons COS + H_2O$$

Similar relationships may also hold for nitrogen species such as ammonia and hydrogen cyanide.

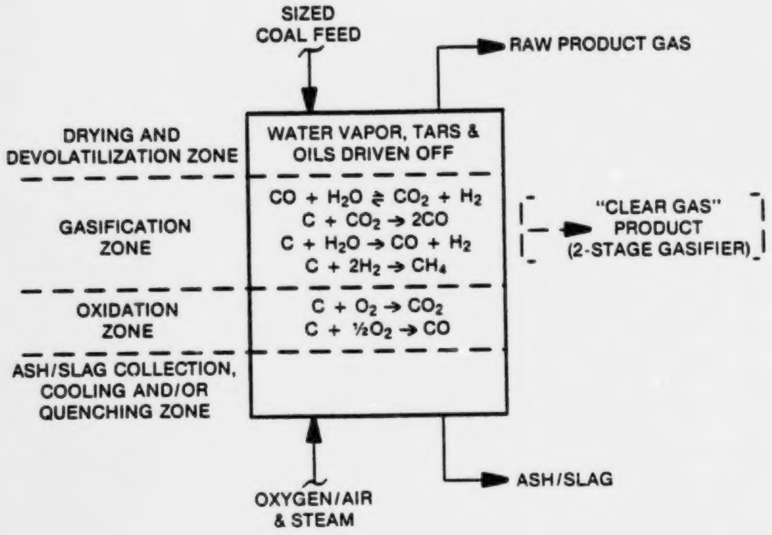
Solid Waste

Coal contains substantial quantities of nonreactive mineral matter which remains after the coal has been gasified. The resulting solid waste will be in the form of ash or solidified slag droplets, depending primarily on the reactor operating temperature and the ash fusion point. Fixed-bed gasifiers can be operated to produce either a "dry", unfused ash (low-temperature operation) or a fused slag by-product (high-temperature operation). Entrained-bed gasifiers operate at high temperatures and produce a slag by-product. Some fluidized-bed gasifiers operate at a temperature at which the ash particles are soft and sticky and form agglomerates that are removed from the gasifier. Some of the mineral matter components may also be volatilized; the extent to which this occurs depends on the temperature and the chemical forms in which these compounds are found in the coal.

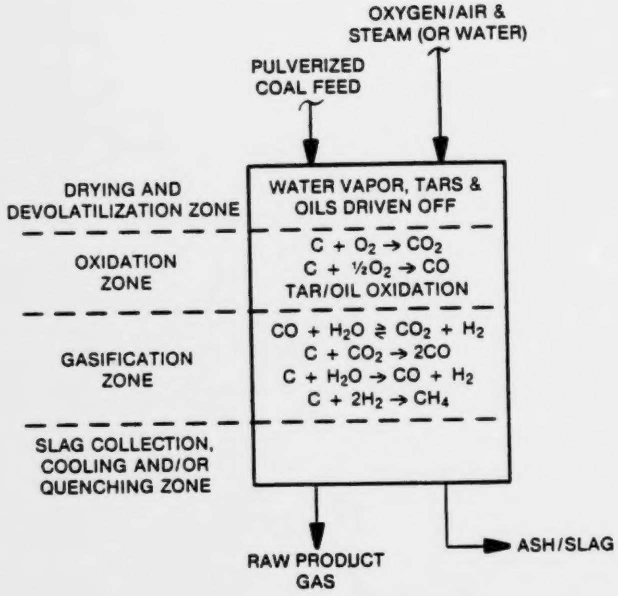
The susceptibility to leaching of the species remaining in the ash or slag is also likely to vary depending on their solubility and the ease with which water can penetrate the solid. For example, fused slags are less subject to leaching than more porous ash particles.

Figure 2 shows the conceptual zones into which fixed-bed, fluidized-bed, and entrained-bed gasifiers may be divided. Note that in the fixed-bed and fluidized-bed gasifiers, the relative direction of gas and solid flows is countercurrent, while it is co-current in the entrained-bed gasifier. Also note the differences in the order of the various reaction zones.

Associated closely with the gasification operation are the equipment and operations required to prepare the coal and feed it into the gasifier


SIZED COAL FEED
RAW PRODUCT GAS
DRYING AND DEVOLATILIZATION ZONE
WATER VAPOR, TARS & OILS DRIVEN OFF
GASIFICATION ZONE
$CO + H_2O \rightleftarrows CO_2 + H_2$
$C + CO_2 \rightarrow 2CO$
$C + H_2O \rightarrow CO + H_2$
$C + 2H_2 \rightarrow CH_4$
"CLEAR GAS" PRODUCT (2-STAGE GASIFIER)
OXIDATION ZONE
$C + O_2 \rightarrow CO_2$
$C + \frac{1}{2}O_2 \rightarrow CO$
ASH/SLAG COLLECTION, COOLING AND/OR QUENCHING ZONE
OXYGEN/AIR & STEAM
ASH/SLAG

FIXED BED,
COUNTERCURRENT GASIFIER


OXYGEN/AIR & STEAM (OR WATER)
PULVERIZED COAL FEED
DRYING AND DEVOLATILIZATION ZONE
WATER VAPOR, TARS & OILS DRIVEN OFF
OXIDATION ZONE
$C + O_2 \rightarrow CO_2$
$C + \frac{1}{2}O_2 \rightarrow CO$
TAR/OIL OXIDATION
GASIFICATION ZONE
$CO + H_2O \rightleftarrows CO_2 + H_2$
$C + CO_2 \rightarrow 2CO$
$C + H_2O \rightarrow CO + H_2$
$C + 2H_2 \rightarrow CH_4$
SLAG COLLECTION, COOLING AND/OR QUENCHING ZONE
RAW PRODUCT GAS
ASH/SLAG

ENTRAINED-BED,
CO-CURRENT GASIFIER

Figure 2. Conceptual configurations of different gasifier bed types.

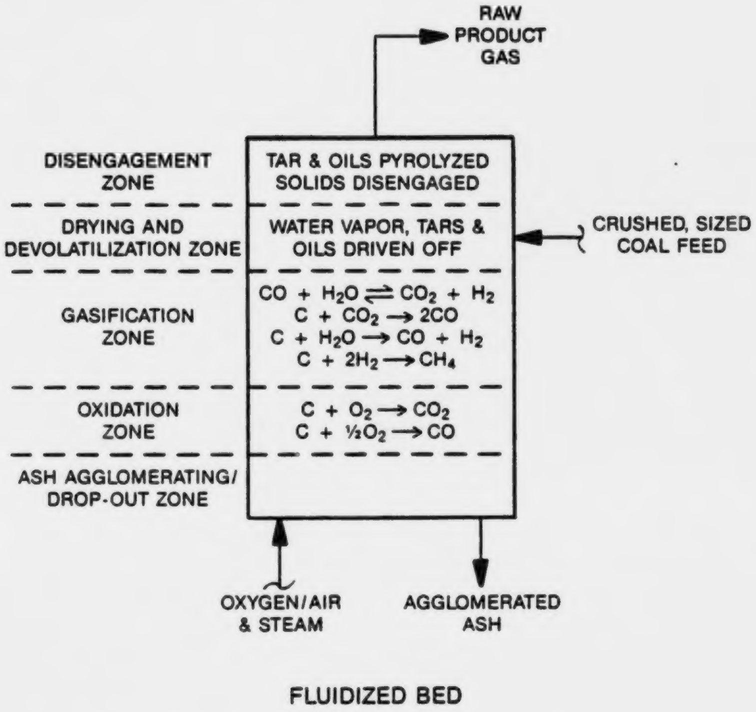

RAW PRODUCT GAS
DISENGAGEMENT ZONE
TAR & OILS PYROLYZED SOLIDS DISENGAGED
DRYING AND DEVOLATILIZATION ZONE
WATER VAPOR, TARS & OILS DRIVEN OFF
CRUSHED, SIZED COAL FEED
GASIFICATION ZONE
$CO + H_2O \rightleftharpoons CO_2 + H_2$
$C + CO_2 \rightarrow 2CO$
$C + H_2O \rightarrow CO + H_2$
$C + 2H_2 \rightarrow CH_4$
OXIDATION ZONE
$C + O_2 \rightarrow CO_2$
$C + \frac{1}{2}O_2 \rightarrow CO$
ASH AGGLOMERATING/ DROP-OUT ZONE
OXYGEN/AIR & STEAM
AGGLOMERATED ASH
FLUIDIZED BED

Figure 2. (Continued)

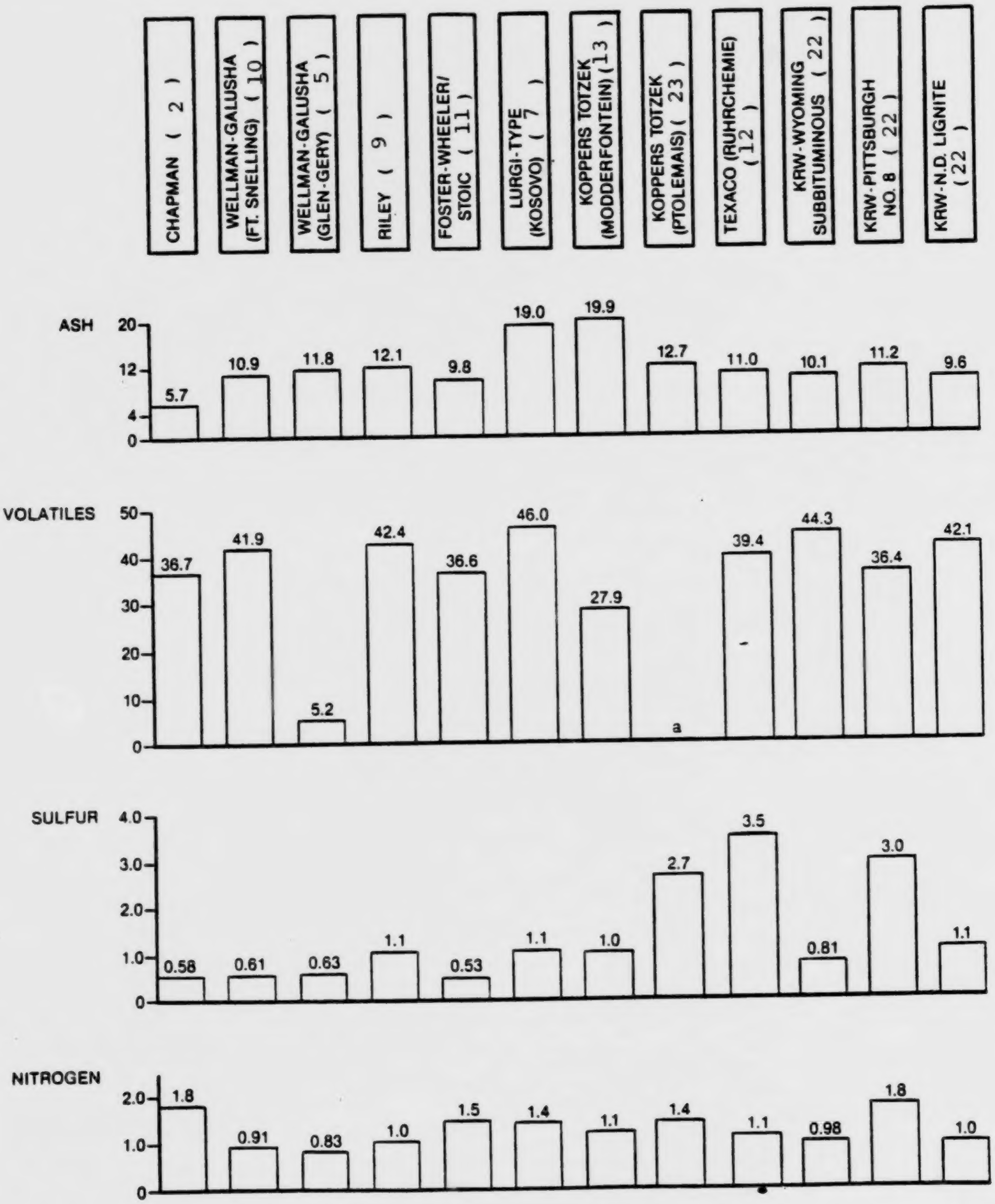
vessels. In the case of most small, low-Btu gasification facilities, very limited coal preparation is performed. These facilities typically gasify coal which has been sized prior to its delivery to the site. Some screening of the coal for removal of fines is performed at two of the low-Btu facilities tested (Wellman-Galusha at Fort Snelling, and Foster-Wheeler/STOIC at UMD). As-received coal is crushed and sized on site at all of the medium-Btu facilities considered in this report. At the Lurgi-type (Kosovo), KRW PDU, and Koppers-Totzek (Modderfontein and Ptolemais) facilities, coal drying is performed. The entrained-bed gasifiers (Koppers-Totzek and Texaco) require more extensive preparation (crushing and pulverizing) to produce the finely divided coal feed used in these gasifiers.

A variety of methods are used to feed the prepared coal into the gasifiers. Lockhoppers are used with Wellman-Galusha, Riley, Foster-Wheeler/STOIC, Lurgi and KRW gasifiers. At the Chapman gasifier facility, coal is fed by means of a rotary feeding device known as a barrel valve. In the GKT gasifier, coal is augered out of a storage vessel and transported to the gasifier in a heated stream of steam and oxygen using a screw conveyor. The Texaco gasifier utilizes a slurry system in which pulverized coal is mixed with water, preheated, and pumped into the gasifier vessel.

Figures 3 through 5 summarize coal composition, gasifier feed rates, and reactant ratios for each of the gasification facilities. Flow rates are shown on a "per gasifier" basis to facilitate comparisons. The reactant ratios were calculated based on the reported feed rates. For the air-blown gasifiers, the oxygen to coal ratio was calculated based on an oxygen content of 23.1 percent by weight for air.

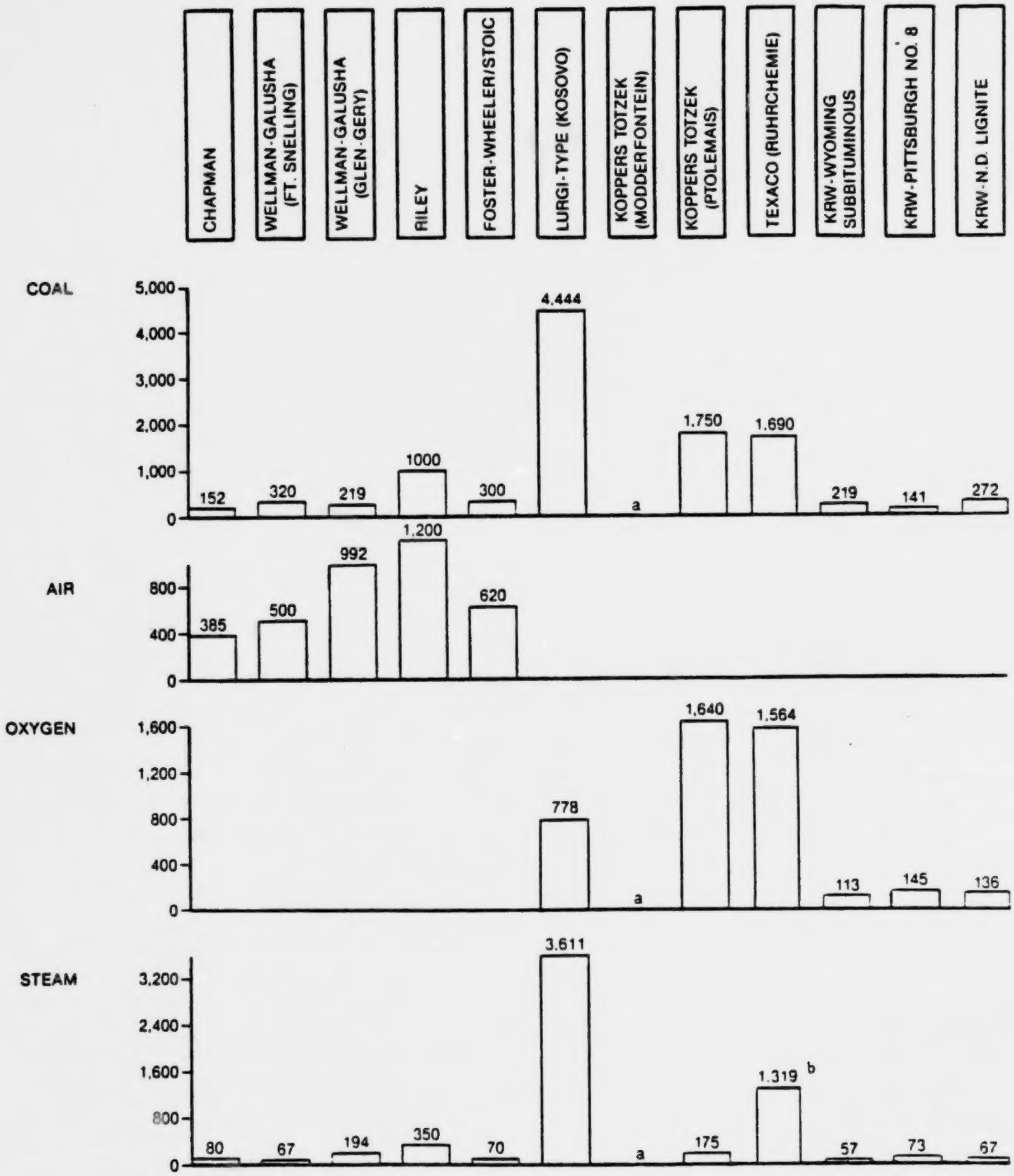
SUMMARY AND COMPARISON OF DOWNSTREAM PROCESSING OPERATIONS

Processing operations downstream of gasification are needed to perform various functions including:



[a] No Data Available.

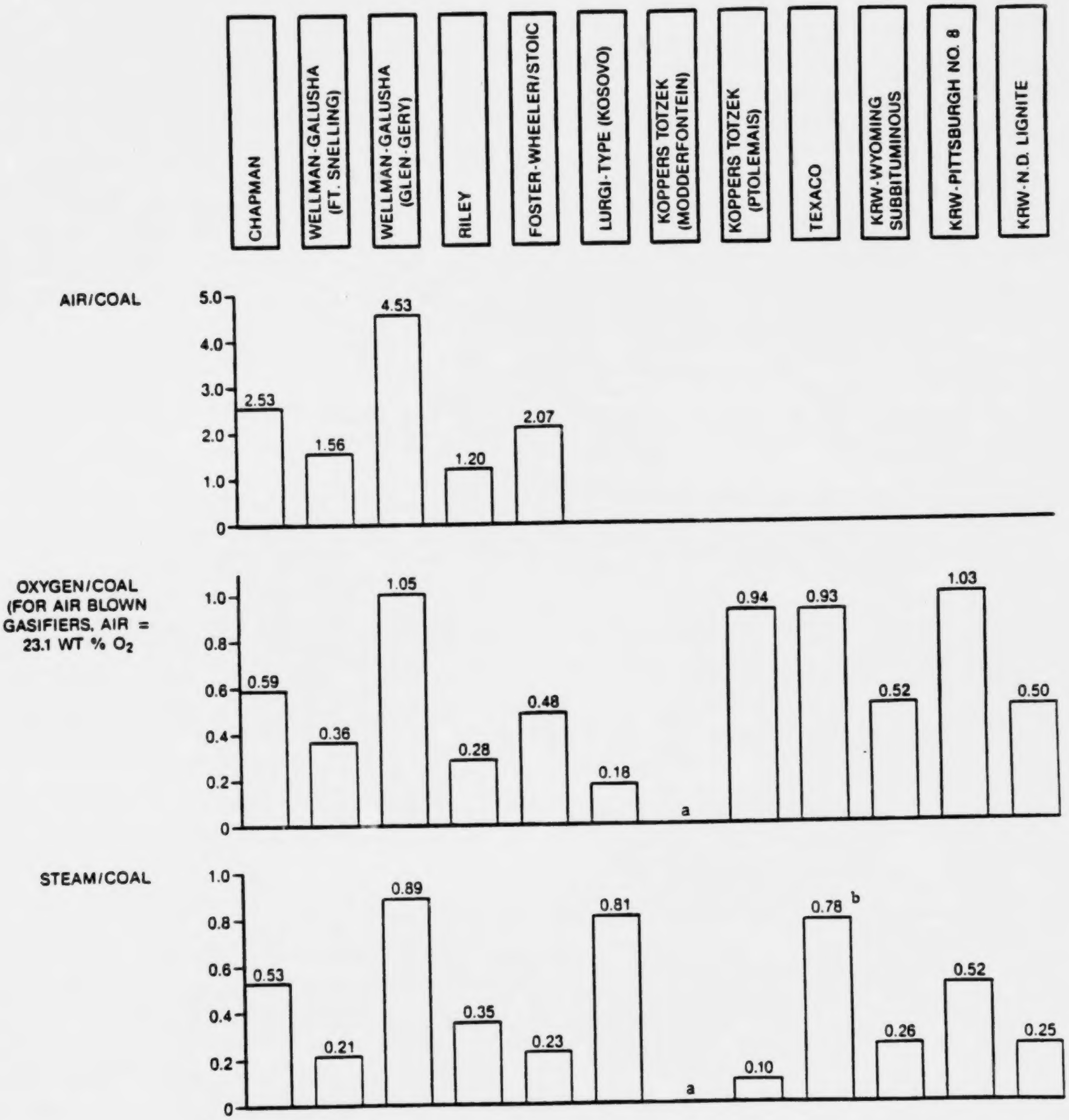
Figure 3. Comparative coal feedstock analyses, dry basis, wt. %.



[a] No data available.

[b] For the Texaco Gasifier Only, the Steam Flow Rate is Taken as the Fresh Makeup Slurry Water, Coal Moisture, and Water in Additive and Flocculant.

Figure 4. Comparative gasifier feed rates, g/sec-gasifier.



[a] No data available.

[b] For the Texaco Gasifier Only, the Steam Flow Rate is Taken as the Fresh Makeup Slurry Water, Coal Moisture, and Water in Additive and Flocculant.

Figure 5. Comparative gasifier feed ratios, kg/kg.

- Removal of entrained particulates (fly ash, tar, oil, etc.),
- Removal of gaseous contaminants (primarily sulfur and nitrogen species),
- Cooling of the raw product gas,
- Handling and disposal of solid wastes,
- Treatment and disposal of wastewater,
- Recovery of by-products (e.g., sulfur, ammonia, organics),
- Control of air pollutants, and
- Upgrading of the raw gas.

All of these processing operations are not present in all gasification facilities. Those found in the gasification facilities included in this report were shown in Table 2. Figures 6 through 15 are simplified block flow diagrams of these facilities. The major processing units and streams present in each of the facilities are shown, together with stream temperature data obtained at the time the facilities were characterized. Those streams for which composition and/or flow rate data were obtained are also indicated. These diagrams clearly show similarities and differences among the facilities.

In general, the low-Btu gasification facilities have much less extensive downstream processing than the larger, more complex medium-Btu facilities. In addition, since the emphasis at the KRW PDU is on gasifier development, limited gas cleaning is practical. In several of the low-Btu facilities, gas cleanup consists only of removing entrained particulates, typically by the use of cyclone separators. This is particularly true of the facilities which produce a hot fuel gas for direct combustion in a process

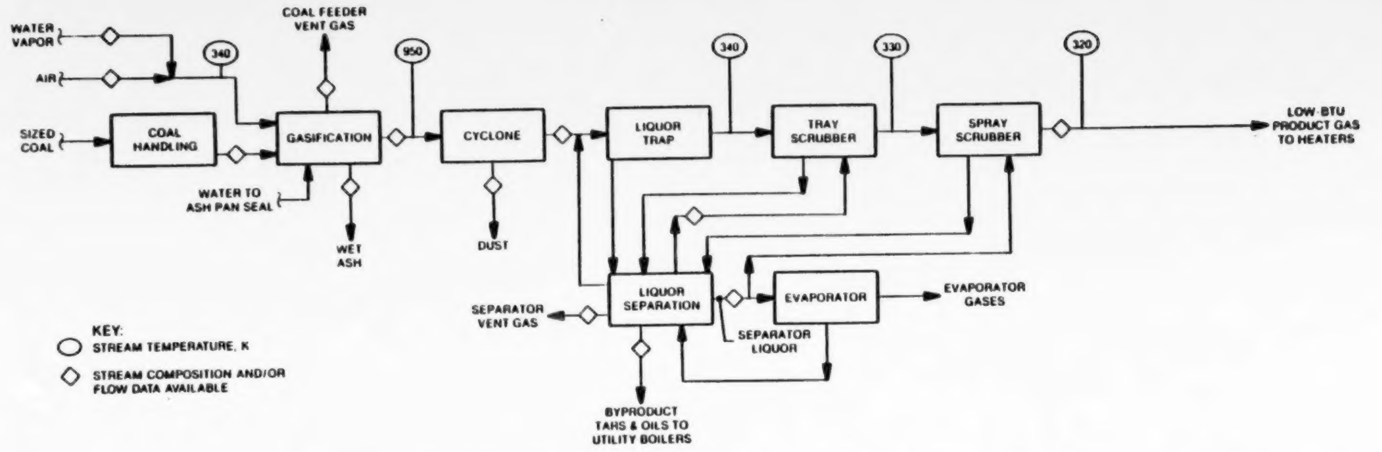

WATER VAPOR
AIR
SIZED COAL
340
COAL HANDLING
COAL FEEDER VENT GAS
GASIFICATION
WATER TO ASH PAN SEAL
WET ASH
950
CYCLONE
DUST
LIQUOR TRAP
340
TRAY SCRUBBER
330
SPRAY SCRUBBER
320
LOW-BTU PRODUCT GAS TO HEATERS
LIQUOR SEPARATION
SEPARATOR VENT GAS
BYPRODUCT TARS & OILS TO UTILITY BOILERS
SEPARATOR LIQUOR
EVAPORATOR
EVAPORATOR GASES
KEY:
STREAM TEMPERATURE, K
STREAM COMPOSITION AND/OR FLOW DATA AVAILABLE

Figure 6. **Simplified block flow diagram of Chapman gasifier.**

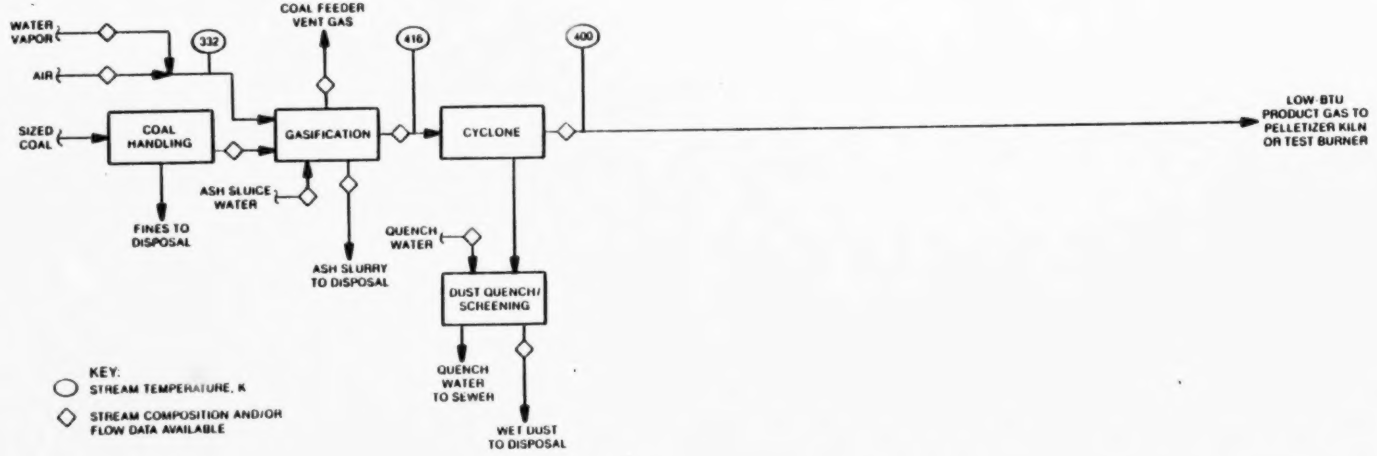

WATER VAPOR
AIR
SIZED COAL
332
COAL HANDLING
FINES TO DISPOSAL
COAL FEEDER VENT GAS
GASIFICATION
ASH SLUICE WATER
ASH SLURRY TO DISPOSAL
416
CYCLONE
400
LOW-BTU PRODUCT GAS TO PELLETIZER KILN OR TEST BURNER
QUENCH WATER
DUST QUENCH/ SCREENING
QUENCH WATER TO SEWER
WET DUST TO DISPOSAL
KEY:
STREAM TEMPERATURE, K
STREAM COMPOSITION AND/OR FLOW DATA AVAILABLE

Figure 7. **Simplified block flow diagram of Wellman-Galusha (Ft. Snelling) gasifier.**

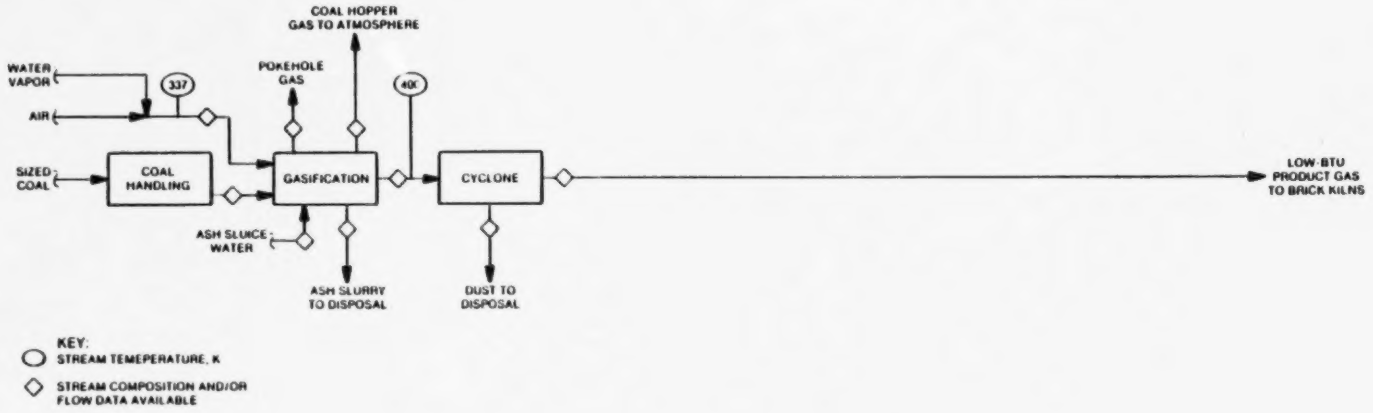

WATER VAPOR
AIR
SIZED COAL
COAL HANDLING
337
POKEHOLE GAS
COAL HOPPER GAS TO ATMOSPHERE
400
GASIFICATION
CYCLONE
ASH SLUICE WATER
ASH SLURRY TO DISPOSAL
DUST TO DISPOSAL
LOW-BTU PRODUCT GAS TO BRICK KILNS
KEY:
STREAM TEMEPERATURE, K
STREAM COMPOSITION AND/OR FLOW DATA AVAILABLE

Figure 8. Simplified block flow diagram of Wellman-Galusha (Glen-Gery) gasifier.

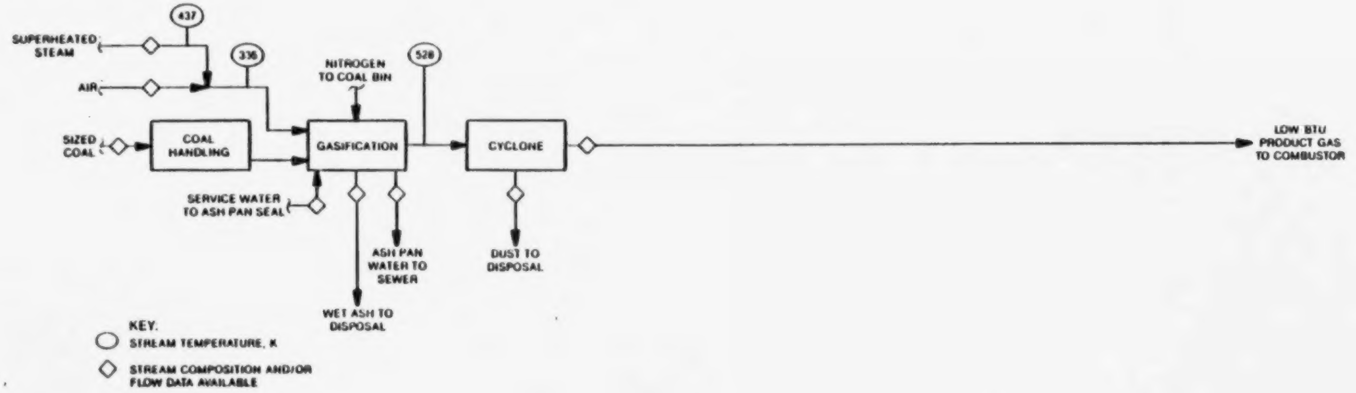

SUPERHEATED STEAM
AIR
SIZED COAL
437
336
COAL HANDLING
NITROGEN TO COAL BIN
528
GASIFICATION
CYCLONE
SERVICE WATER TO ASH PAN SEAL
ASH PAN WATER TO SEWER
WET ASH TO DISPOSAL
DUST TO DISPOSAL
LOW BTU PRODUCT GAS TO COMBUSTOR
KEY:
STREAM TEMPERATURE, K
STREAM COMPOSITION AND/OR FLOW DATA AVAILABLE

Figure 9. Simplified block flow diagram of Riley gasifier.

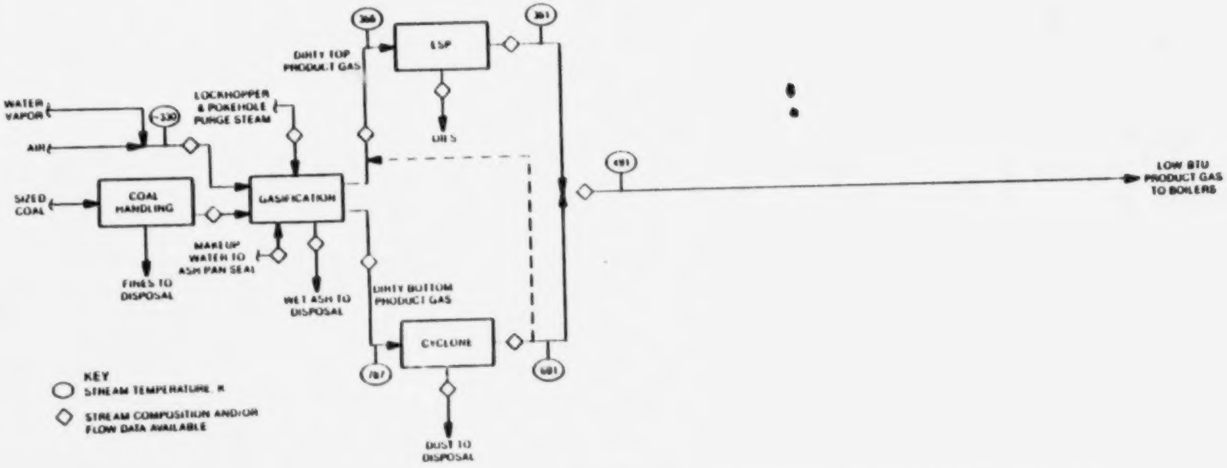

WATER VAPOR
AIR
SIZED COAL
~330
COAL HANDLING
FINES TO DISPOSAL
LOCKHOPPER & POKEHOLE PURGE STEAM
GASIFICATION
MAKEUP WATER TO ASH PAN SEAL
WET ASH TO DISPOSAL
DIRTY TOP PRODUCT GAS
ESP
OILS
DIRTY BOTTOM PRODUCT GAS
CYCLONE
787
DUST TO DISPOSAL
491
LOW BTU PRODUCT GAS TO BOILERS
KEY
STREAM TEMPERATURE, K
STREAM COMPOSITION AND/OR FLOW DATA AVAILABLE

Figure 10. Simplified block flow diagram of Foster-Wheeler/STOIC gasifier.

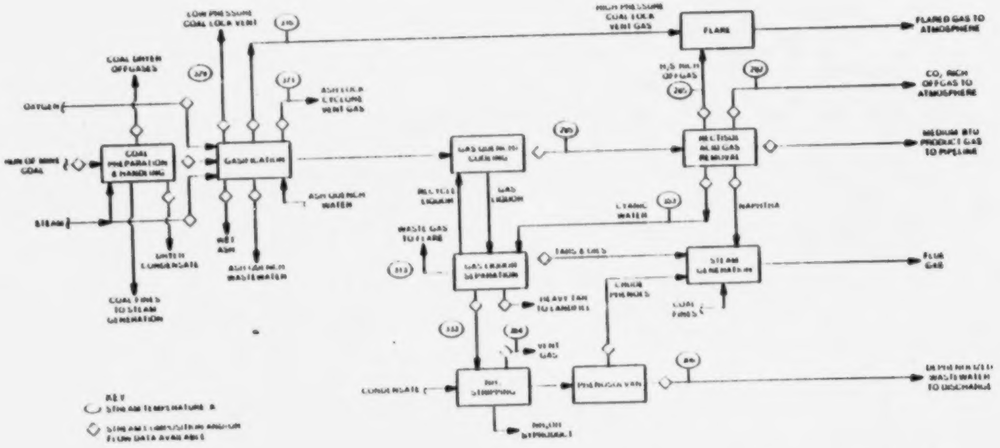

OXYGEN
COAL DRYER OFFGASES
STEAM
COAL PREPARATION & HANDLING
COAL FINES TO STEAM GENERATION
GASIFICATION
WET ASH
LOW PRESSURE COAL LOCK VENT
ASH LOCK CYCLONE VENT GAS
ASH QUENCH WATER
HIGH PRESSURE COAL LOCK VENT GAS
FLARE
FLARED GAS TO ATMOSPHERE
RECYCLE LIQUOR
GAS LIQUOR
WASTE GAS TO FLARE
HEAVY TAR TO LANDFILL
VENT GAS
CONDENSATE
STRIPPING
H_2S RICH OFFGAS
CO_2 RICH OFFGAS TO ATMOSPHERE
RECTISOL ACID GAS REMOVAL
MEDIUM BTU PRODUCT GAS TO PIPELINE
NAPHTHA
TARS & OILS
STEAM GENERATION
FLUE GAS
COAL FINES
DEPHENOLIZED WASTEWATER TO DISCHARGE
KEY
STREAM TEMPERATURE, K
STREAM COMPOSITION AND/OR FLOW DATA AVAILABLE

Figure 11. Simplified block flow diagram of Lurgi-type gasifier.

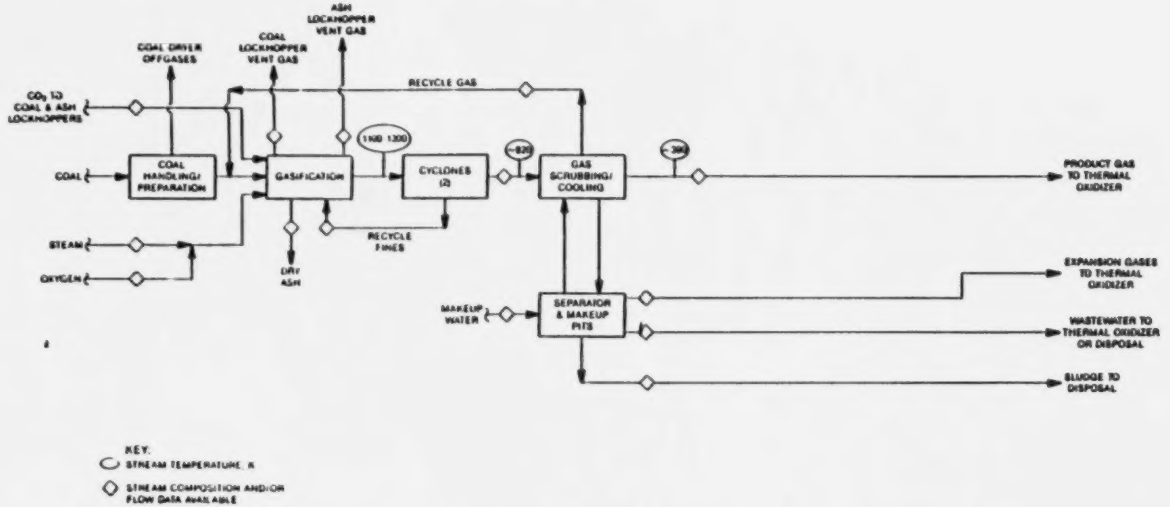

CO2 1,3
COAL & ASH
LOCKHOPPERS
COAL
STEAM
OXYGEN
COAL DRYER
OFFGASES
COAL
HANDLING/
PREPARATION
COAL
LOCKHOPPER
VENT GAS
ASH
LOCKHOPPER
VENT GAS
RECYCLE GAS
GASIFICATION
1100-1300
CYCLONES
(2)
~820
GAS
SCRUBBING/
COOLING
~390
DRY
ASH
RECYCLE
FINES
MAKEUP
WATER
SEPARATOR
& MAKEUP
PITS
PRODUCT GAS
TO THERMAL
OXIDIZER
EXPANSION GASES
TO THERMAL
OXIDIZER
WASTEWATER TO
THERMAL OXIDIZER
OR DISPOSAL
SLUDGE TO
DISPOSAL
KEY:
STREAM TEMPERATURE, K
STREAM COMPOSITION AND/OR
FLOW DATA AVAILABLE

Figure 12. Simplified block flow diagram of KRW PDU gasifier.

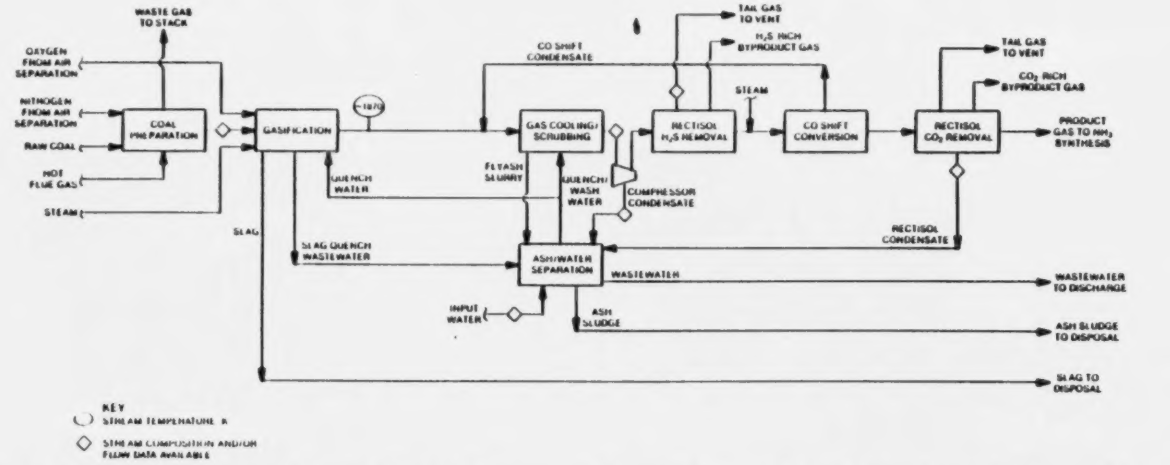

WASTE GAS
TO STACK
OXYGEN
FROM AIR
SEPARATION
NITROGEN
FROM AIR
SEPARATION
RAW COAL
HOT
FLUE GAS
STEAM
COAL
PREPARATION
GASIFICATION
~1870
SLAG
QUENCH
WATER
SLAG QUENCH
WASTEWATER
CO SHIFT
CONDENSATE
FLYASH
SLURRY
GAS COOLING/
SCRUBBING
QUENCH/
WASH
WATER
COMPRESSOR
CONDENSATE
RECTISOL
H2S REMOVAL
TAIL GAS
TO VENT
H2S RICH
BYPRODUCT GAS
STEAM
CO SHIFT
CONVERSION
RECTISOL
CO2 REMOVAL
TAIL GAS
TO VENT
CO2 RICH
BYPRODUCT GAS
PRODUCT
GAS TO NH3
SYNTHESIS
RECTISOL
CONDENSATE
ASH/WATER
SEPARATION
WASTEWATER
INPUT
WATER
ASH
SLUDGE
WASTEWATER
TO DISCHARGE
ASH SLUDGE
TO DISPOSAL
SLAG TO
DISPOSAL
KEY
STREAM TEMPERATURE, K
STREAM COMPOSITION AND/OR
FLOW DATA AVAILABLE

Figure 13. Simplified block flow diagram of Koppers-Totzek (Modderfontein) gasifier.

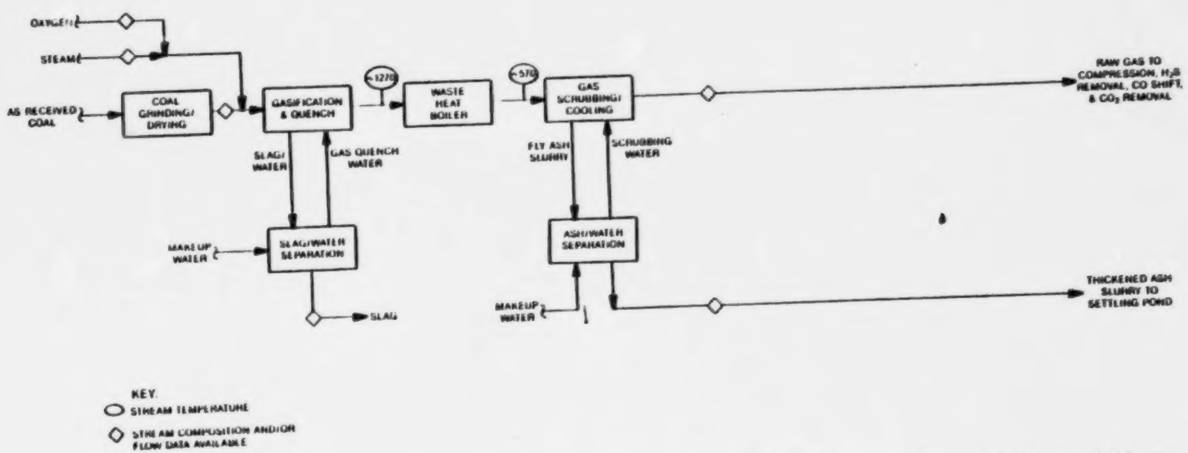

OXYGEN
STEAM
AS RECEIVED COAL
COAL GRINDING/ DRYING
GASIFICATION & QUENCH
~1270
WASTE HEAT BOILER
~570
GAS SCRUBBING/ COOLING
RAW GAS TO COMPRESSION, H2S REMOVAL, CO SHIFT, & CO2 REMOVAL
SLAG/ WATER
GAS QUENCH WATER
FLY ASH SLURRY
SCRUBBING WATER
MAKEUP WATER
SLAG/WATER SEPARATION
ASH/WATER SEPARATION
MAKEUP WATER
SLAG
THICKENED ASH SLURRY TO SETTLING POND
KEY
STREAM TEMPERATURE
STREAM COMPOSITION AND/OR FLOW DATA AVAILABLE

Figure 14. Simplified block flow diagram of Koppers-Totzek (Ptolemais) gasifier.

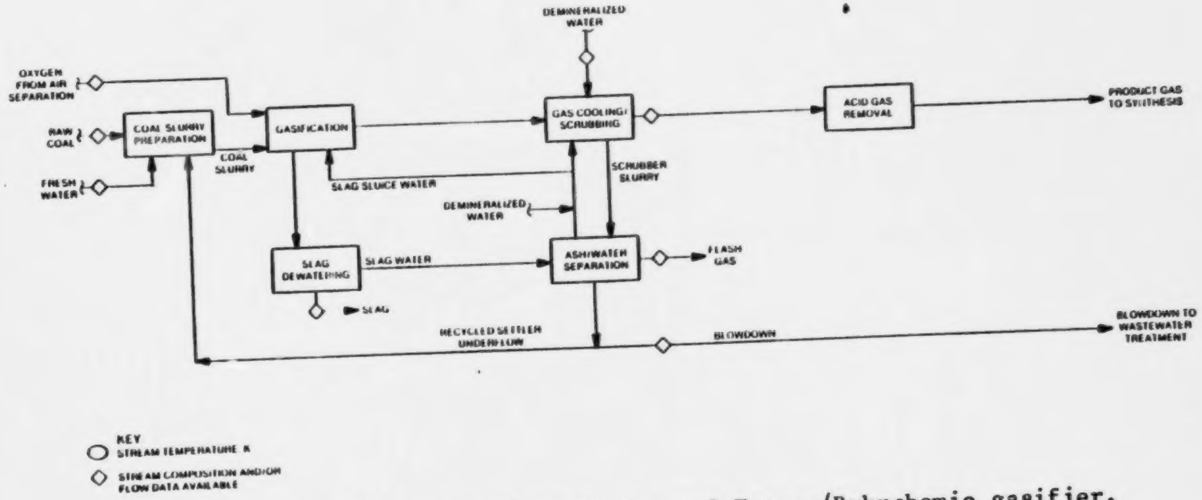

DEMINERALIZED WATER
OXYGEN FROM AIR SEPARATION
RAW COAL
FRESH WATER
COAL SLURRY PREPARATION
COAL SLURRY
GASIFICATION
GAS COOLING/ SCRUBBING
ACID GAS REMOVAL
PRODUCT GAS TO SYNTHESIS
SLAG SLUICE WATER
SCRUBBER SLURRY
DEMINERALIZED WATER
SLAG DEWATERING
SLAG WATER
ASH/WATER SEPARATION
FLASH GAS
SLAG
RECYCLED SETTLER UNDERFLOW
BLOWDOWN
BLOWDOWN TO WASTEWATER TREATMENT
KEY
STREAM TEMPERATURE K
STREAM COMPOSITION AND/OR FLOW DATA AVAILABLE

Figure 15. Simplified block flow diagram of Texaco/Ruhrchemie gasifier.

furnace. The Foster-Wheeler/STOIC facility (which features two-stage gasification) utilizes an electrostatic precipitator (ESP) to remove oil and tar particulates from the top gas and a cyclone to remove dust from the bottom gas. Of the low-Btu gasifiers tested, only the Chapman facility utilizes wet scrubbing and produces a cooled fuel gas, by-product tars and oils, and a process condensate (wastewater) stream. Some type of wet scrubbing is used in all of the medium-Btu facilities. None of the low-Btu facilities have acid gas removal systems; all of the commercial medium-Btu facilities have such units.

Ash/slag removal techniques also vary. All of the facilities except the KRW PDU use water to quench the hot ash/slag or to facilitate its removal from the gasifier vessel by sluicing. The pressurized gasifiers (Lurgi, KRW, and Texaco) all utilize lock hoppers to remove ash/slag. The others utilize ash plows, mechanical conveyors, or slide valves.

The downstream processing operations can significantly influence the fates of the various solid, liquid, and gaseous pollutants generated in the gasifier. Components originally found in the raw gas may be removed by these operations and distributed into a number of secondary solid, liquid, or gaseous streams. This distribution depends on the way in which these processes are linked together, how they are designed and operated, and on stream compositions.

Flow rate data for the major streams entering and leaving the downstream processing units for each of the facilities considered are summarized in Appendix A.

SECTION 4

SAMPLING AND ANALYSIS TECHNIQUES

The sampling and analysis methods that were used to characterize the organics in the various coal gasification processes were test-specific; however, the same basic principles were employed throughout. Therefore, a simplified methodology that represents these basic principles is given here to describe how the condensable organics were obtained and how they were analyzed.

SAMPLING METHODS

The sampling method descriptions are grouped by stream type (i.e., gas, liquid, and solid). Gas stream sampling was the most complex and required the major portion of the sampling effort.

Gas Streams

Gas streams were sampled by means of a train consisting of two parts:

- a probe and nozzle system to extract the sample from the gas stream and
- a collection train to cool the gas, retain the condensate, and collect the vapor phase organics on sorptive resin (generally XAD-2).

Gas streams with a high moisture content, above 50% by volume, were sampled with additional empty impingers placed upstream of the normal condensor to remove excess condensate and provide additional gas cooling.

Material for analysis was recovered from the probe and sample line with a methylene chloride rinse. The aqueous portion of the condensate was separated and stored. Remaining organic material from the collection train and connecting glassware was recovered with a methylene chloride rinse which was then combined with the probe rinse. The XAD-2 resin containing the sorbed hydrocarbons was transferred to the original resin container.

In many tests, the EPA Source Analysis Sampling System (SASS) Train was used. This system follows the same principle and collection technique described above. For the details of the specific sampling and analysis methodologies, it is recommended that the appropriate source test report be consulted.

Liquid Samples

Liquid samples were generally collected either with a dipper from streams with an open hatchway or from a spigot. Sample containers appropriate for each of the planned analytical techniques were filled completely to minimize the entrainment of air.

Solid Samples

Grab samples usually were collected from ash and coal transfer systems. Heavy tars were collected as liquids and allowed to solidify.

ANALYTICAL METHODS

The methods used to characterize organics are based on recognized analytical techniques such as gas chromatography, liquid chromatography, GC-MS, and chemical analyses. The methodology was based primarily on the U.S. EPA protocol for a Level 1 source assessment (18) and methods for water quality analyses.

Preparation of Samples for Organic Analysis

This section addresses the general sample preparation technique for condensed vapors, liquids, and solids. Once prepared or extracted, the analysis of each extract type was the same. The types of samples prepared for organic analysis were:

- condensable organics sorbed on XAD-2 resin,
- organic condensates in methylene chloride,
- aqueous liquids,
- solids, and
- by-products.

A sample may have extracts from two or more of the above classifications. If so, these extracts were prepared individually then composited to form a single sample for organic analysis. The extraction and preparation procedures for each type of sample or matrix are discussed below.

XAD-2 Resin--

A porous polymer resin (XAD-2) was used to sorb vapor phase organics from gas streams. Prior to sampling, the resin was cleaned to reduce background interferences which would be extracted during sample recovery. Blanks were used to correct for any organic material which was extracted from the clean resin during sample recovery. The organics sorbed (or condensed) during sampling were recovered from the resin by extraction with methylene chloride (CH_2Cl_2). Extracted organics were most often separated into two fractions, one containing acids and the other containing base/neutrals, by liquid partitioning between the solvent and aqueous base. The resulting acid and base/neutral fractions were combined then with other like fractions from other portions of the same sample if appropriate. A typical extraction flow scheme for the resin is given in Appendix B (Figure B-1).

Organic Condensates in Methylene Chloride--

Recovery of a gas sample included a rinse of the sampling train with CH_2Cl_2. This rinse removed organics and particulates coating the interior walls of the train. This recovered material was eventually combined with the extracts of the same sample. Acid and base/neutral fractions were separated by back extraction as done for the resin. A generic scheme for this preparative step is given in Appendix B (Figure B-2).

Particulates contained in the rinse were quantified by determining the residue gravimetrically after filtration. Condensable tars and oils were quantified by determining the residue after evaporation. These results were combined with the filterable and dissolved solids from the aqueous portion of the impinger solutions to determine the total particulate catch.

Aqueous Liquids--

The aqueous and non-aqueous phases of liquid samples were separated. The aqueous phase was extracted with CH_2Cl_2 after pH adjustment. The organic phase was dissolved in methylene chloride and subjected to the acid and base/neutral extraction scheme. The resulting base/neutral and acid fractions were combined with other like fractions for subsequent analyses. Details of the separation and extractions are given in Appendix B (Figure B-3).

Solids--

A known weight of solid sample was transferred to a soxhlet thimble, weighed, and extracted with CH_2Cl_2 for 24 hours. The extract generally was back extracted to generate base/neutral and acid fractions as was done for the XAD-2 resin. Solids remaining after extraction were reweighed to determine the percent extractables present in the sample. This preparation scheme is the same as shown for XAD-2 in Appendix B (Figure B-1).

By-Products--

The organic liquids were diluted with a known volume of CH_2Cl_2 and then filtered to remove particulates and other insoluble matter. The CH_2Cl_2 then was back extracted to generate the base/neutral and acid fractions for introduction into the remainder of the analytical scheme. This preparation scheme is shown in Appendix B (Figure B-5).

Analysis of Organic Loading

Organic extracts from the various preparatory steps were combined and analyzed by the EPA protocol (18) for total chromatographable organics (TCO) and gravimetrically determined organics (GRAV) following the strategy diagrammed in Figure 16. Samples meeting the quantity criteria defined in the strategy were fractionated by column liquid chromatography to characterize the mass distribution according to chromatographic retention (Appendix C, Figure C-1). Procedures for these determinations are summarized below.

Total Chromatographable Organics (TCO)--

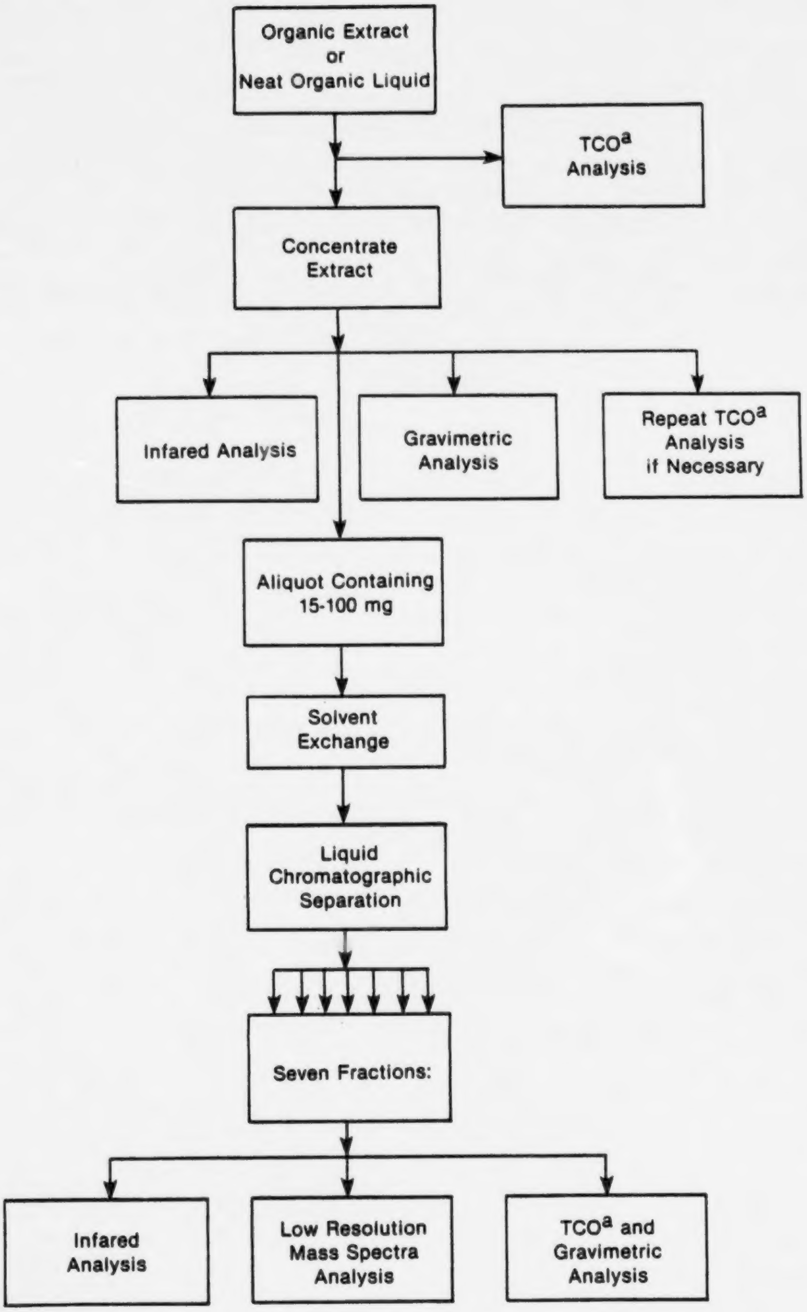
The total chromatographable organics determination quantifies the materials with boiling points in the range of 100 to 300°C. The determination is made by gas chromatography using a flame ionization detector and a 1.8m x 3 mm O.D. stainless steel column packed with 10% OV 101 on 100/120 Supelcoport (or an equivalent).

Gravimetrically Determined Organics (GRAV)--

Components with boiling points higher than 300°C were determined gravimetrically. The determinations are made after the extract has been properly concentrated to a level that will yield a weighable residue from a 1 mL aliquot. Final evaporation is carried out at room temperature in still air until constant weight is achieved.

Liquid Chromatographic Separation--

The Liquid Chromatographic Separation is made on an aliquot of a previously prepared sample containing between 15 and 100 mg of organic material. Components are separated on a column of activated silica gel using an elution sequence of solvents of increasing polarity from pentane to 1:1 methylene


Organic Extract
or
Neat Organic Liquid
TCO[a] Analysis
Concentrate Extract
Infared Analysis
Gravimetric Analysis
Repeat TCO[a] Analysis if Necessary
Aliquot Containing 15-100 mg
Solvent Exchange
Liquid Chromatographic Separation
Seven Fractions:
Infared Analysis
Low Resolution Mass Spectra Analysis
TCO[a] and Gravimetric Analysis

[a] TCO analyses are not necessary for samples for which process or collection temperatures were 200°C (400°F) or higher.

Figure 16. Organic analysis methodology.

chloride and methanol as listed in Appendix B. After each fraction is collected, a 5 uL aliquot is taken for the TCO determination, and the balance is used for the GRAV determination after which IR is run on the residue.

Detailed Organic Analyses

Detailed analyses of organic extracts and LC fractions were done primarily by gas chromatography (GC) and gas chromatography-mass spectrometry (GC-MS). The GC-MS methods varied considerably over the course of the data acquisition programs. Therefore, brief descriptions of several procedures are included to illustrate the extent of procedure variations. Specific techniques used for the tar-producing gasifiers are given in Appendix B.

Determination of Selected Compounds by SIM/GC-MS--

The selective ion monitoring (SIM) technique was employed for many GC-MS analyses. The intensities of key ions were monitored during the chromatographic separation. Identification of a selected compound was based on the appearance of its key ions at a previously established retention time. A second criterion for identification was the relative intensity of the secondary ion of each compound matching within 20% of the intensity found from the analysis of a standard. Quantification was achieved by integration of the areas under the intensity profiles of a key ion for each component. These were compared to the mass and area under the intensity profile of a series of standards at varying concentrations.

Determination of PNAs by GC-MS--

Concentrated extracts prepared as described earlier in this section were analyzed for selected polynuclear aromatics (PNAs) by GC-MS using specific ion monitoring (SIM). The selected compounds generally included benz(a)anthracene, benzo(a)pyrene, benzo(a)fluoranthene, dibenz(a,h)anthracene, and 7,12-dimethylbenz(a)anthracene. A Hewlett-Packard 5982A GC-MS equipped with a liquid crystal column was used for these analyses. The liquid crystal N,N'bis-(p-phenylbenzylidene)2-2'-bi-p-toluidine (BPhBT) gave the necessary separation of PNAs.

Gas Chromatography for Special Analyses

Gas chromatography with a Hall electrolytic conductivity detector (HECD) and with a flame ionization detector (FID) was used as a characterization tool to obtain profiles of the various organic samples and fractions. The FID was used to provide profiles of all gas chromatographable organics while the HECD was used to provide profiles of the sulfur-, the nitrogen-, or the chlorine-bearing hydrocarbons. Other special detectors used in these studies included a flame photometric detector used in the sulfur-specific mode and an electron capture detector to detect halogenated organics.

SECTION 5

RESULTS AND DISCUSSION

COMPARISON OF ORGANIC PRODUCTION RATES

This section compares the organic production rates of the five gasifiers studied that will yield tar when operated with an appropriate feed coal. Table 3 shows the organic condensable loadings and organic mass flow rates of the streams tested. As shown, gasifiers without some form of purification carry higher organics concentrations in the product gas. For example, half of the organics from the Foster-Wheeler/STOIC gasifier are removed as ESP oil, and at least 85% of the organics from the Chapman gasifier are removed as tar.

Table 4 provides estimates of total condensable organics produced per metric ton of coal. The total organic production rate of approximately 200 g/gasifier-second for the Lurgi-type (Kosovo) facility was based on the by-product production rate prior to gas cooling and quenching. This tabulation indicates that these five fixed-bed gasifiers produce comparable amounts of organics with operation on coals with similar levels of volatile matter. Within the limits of error, all values are similar and are close to 30 kg organics/ton of coal.

The objective of this report is not only to summarize production but also to describe the organic composition of the process and discharge streams of these coal gasification plants. Since the data are not uniform across the plants, the formats used here have been adapted to suit the available data. The report considers two major aspects of the concern about organics in coal gasifier discharges: the organic loading of the process streams and the nature and composition of the organics contributing to that loading.

TABLE 3. CONDENSABLE ORGANIC LOADING AND ORGANIC MASS FLOW RATE SUMMARY

	Organic Loading	Organics Mass Flow (g/sec)
Foster-Wheeler/STOIC		
Plant Total		7.5 E0[a]
Ash pan water	1.3 E3 ug/L	9.0 E-6
Cyclone dust	1.2 E2 ug/g	2.4 E-5
Gasifier ash	1.0 E2 ug/g	3.5 E-3
ESP oil	9.3 E5 ug/g	3.7 E0
Combined product gas	4.0 E6 ug/g	3.8 E0
Wellman-Galusha (Ft. Snelling)		
Plant Total		8.7 E0
Gasifier ash	6.4 E2 ug/g	1.5 E-2
Cyclone dust	1.3 E4 ug/g	4.9 E-4
Ash sluice water	1.3 E5 ug/L	<9.0 E-4
Cyclone dust quench water	6.0 E4 ug/L	<4.0 E-4
Product gas composite	1.6 E7 ug/m^3	8.6 E0
Riley		
Plant Total		2.2 E1
Product gas total	9.1 E6 ug/Nm^3	8.0 E0
Product gas aerosols	3.3 E6 ug/Nm^3	-
Product gas vapors	5.8 E6 ug/Nm^3	1.4 E1
Gasifier ash	2.4 E2 ug/g	1.8 E-2
Cyclone dust	5.6 E3 ug/g	2.2 E-2
Ash pan water	1.2 E4 ug/L	2.6 E-2
Chapman		
Plant Total		1.8 E1
Measured total discharges, (excluding by-product tar)		2.6 E0
Product gas	2.4 E6 ug/m^3	1.0 E0
Coal feeder vent	2.4 EG ug/m^3	6.5 E-2
Separator vent	4.2 E6 ug/m^3	2.5 E0
Gasifier ash	1.8 E1 ug/g	1.6 E-4
Cyclone dust	3.8 E2 ug/g	2.6 E0
Tar, by-product	--	1.5 E1

(Continued)

TABLE 3. (Continued)

	Organic Loading	Organics Mass Flow (g/sec)
Lurgi-Type (Kosovo)		
Plant Total		4.1 E1
Total Gas Streams, (excluding start-up vent)		7.8 E0
LP coal lock vent	7.7 E6 ug/m^3	4.5 E-2
HP coal lock vent	2.9 E6 ug/m^3	1.8 E-1
Start-up vent	9.7 E6 ug/m^3	3.4 E-1
H_2S rich waste gas	1.3 E5 ug/m^3	1.3 E-1
CO_2 rich waste gas	1.4 E4 ug/m^3	1.4 E-2
Tar tank vent	1.4 E7 ug/m^3	2.2 E-3
Medium oil tank vent	2.1 E7 ug/m^3	1.0 E-2
Tar separation waste gas	3.3 E6 ug/m^3	2.6 E-2
Phenolic water tank	1.2 E8 ug/m^3	1.9 E-1
Ammonia stripper vent	9.9 E7 ug/m^3	7.2 E0
Naphtha storage tank vent	5.6 E6 ug/m^3	5.9 E-3
Phenosolvan wastewater	1.5 E6 ug/L	5.4 E0
Phenolic water	1.1 E7 ug/L	4.0 E1

[a] 7.5E0 equals 7.5 x 10^0.

TABLE 4. TOTAL CONDENSABLE ORGANIC PRODUCTION BASED ON GAS LOADING AND BY-PRODUCT YIELD

Gasifier	Total Condensable Organics (g/sec)	Coal Feed Rate (g/sec)	Organics/Feed Coal (kg/ton)
Wellman-Galusha (Ft. Snelling)	8.7	250	35
Foster-Wheeler/STOIC	7.5	270	28
Riley	22	670	33
Lurgi-Type (Kosovo)	200[a]	4400	45
Chapman[b]	18[a]	300	60

[a] The values shown are based on production levels of condensable organic by-products. If based on stream analyses then the Kosovo LP-coal lock vent emits 44 g/sec representing 9.9 kg/ton of coal and the Chapman coal feeder vent emits 2.1 g/sec representing 6.9 kg/ton of coal.

[b] Chapman coal feed rate is based on two trains at 150 g/sec each.

The data are broken down into categories and will be discussed in the order listed.

- Organic loading
  - volatile vs. nonvolatile organics
  - liquid chromatographic characterization of total organics (TO)

- Water quality parameters

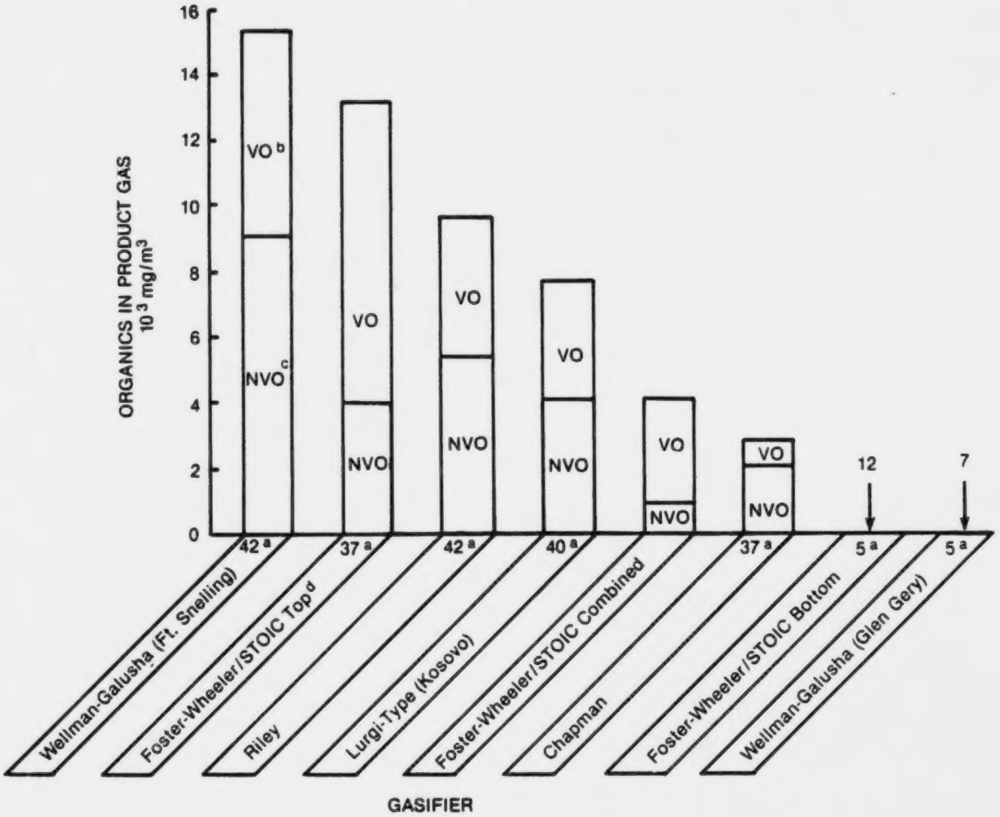
- Detailed organic analyses
  - GC-MS characterization results
  - GC characterization results
  - IR results for extracted organics and LC fractions
  - Low Resolution Mass Spectrometric (LRMS) results

ORGANIC LOADINGS

The organic loadings and characterizations as determined by the EPA-AEERL protocol for a Level 1 environmental assessment (18) are presented for gas, aqueous, and solid phase streams in the sections that follow.

Organic Loadings in Product Gas

The extractable organic loadings in product gas from several tar-producing gasifiers are compared in Figure 17. The figure shows that the crude product gas from the Wellman-Galusha gasifier at the Fort Snelling facility contained the highest loading of volatiles. However, the difference in the loadings was not large among any of the tar-producing gasifiers except for the Wellman-Galusha at Glen Gery, which was operated on anthracite and, therefore, omitted from Tables 3 and 4. The organic loading of top gas from the Foster-Wheeler/STOIC two-stage gasifier was comparable to others, but after passage through the electrostatic precipitator and combination with the bottom gas, the loading was reduced to about 25% of the norm for other gasifiers.



[a] = Percent Volatiles in Feed Coal.
[b] VO = Volatile.
[c] NVO = Non-Volatile.
[d] Foster-Wheeler gasifier is two-stage, fixed bed, fed at top.

Figure 17. Organic loading in product gas from tar-producing gasifiers.

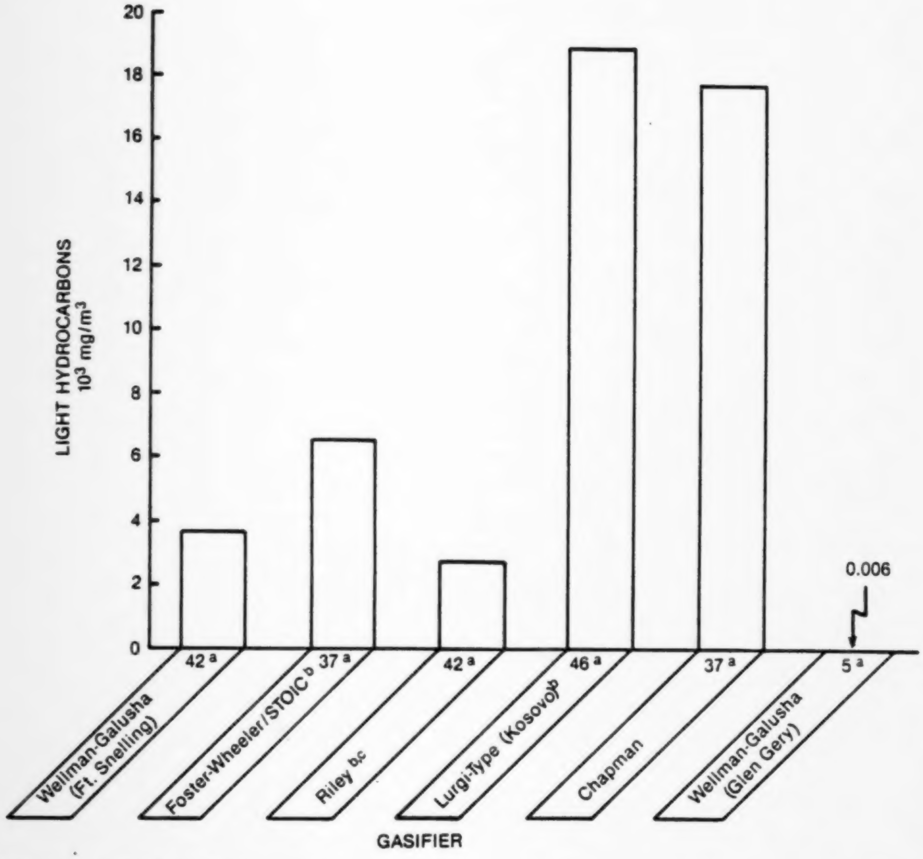
Light hydrocarbons in the product gases are shown as the sum of C_2-C_6 in Figure 18. Although a uniform protocol was not followed for all these GC analyses (e.g., C_5 and C_6 were not determined in the Riley product gas, and benzene, toluene, and xylene were not determined in the Chapman product gas), the combined results indicate the range of light hydrocarbon loadings produced. These results show little apparent correlation with the total organic production levels or the amount of condensable organics measured in the product gas. Detailed data from which these figures were produced are found in Appendix C; organic production rates normalized on coal feed rates are abstracted from these appended tables and compiled below.

TABLE 5. ORGANIC PRODUCTION RATES

Gasifier	Coal Volatile %	Product Gas Kg Organics/ton Coal Consumed	Product Gas Kg Hydrocarbons/ton Coal Consumed
Wellman-Galusha (Ft. Snelling)	42	34	8
Foster-Wheeler/STOIC	32	16	24
Riley	42	30	0
Lurgi-type (Kosovo)	46	10	24
Chapman	37	7	52
Wellman-Galusha (Glen Gery)	5	0.004	0.03

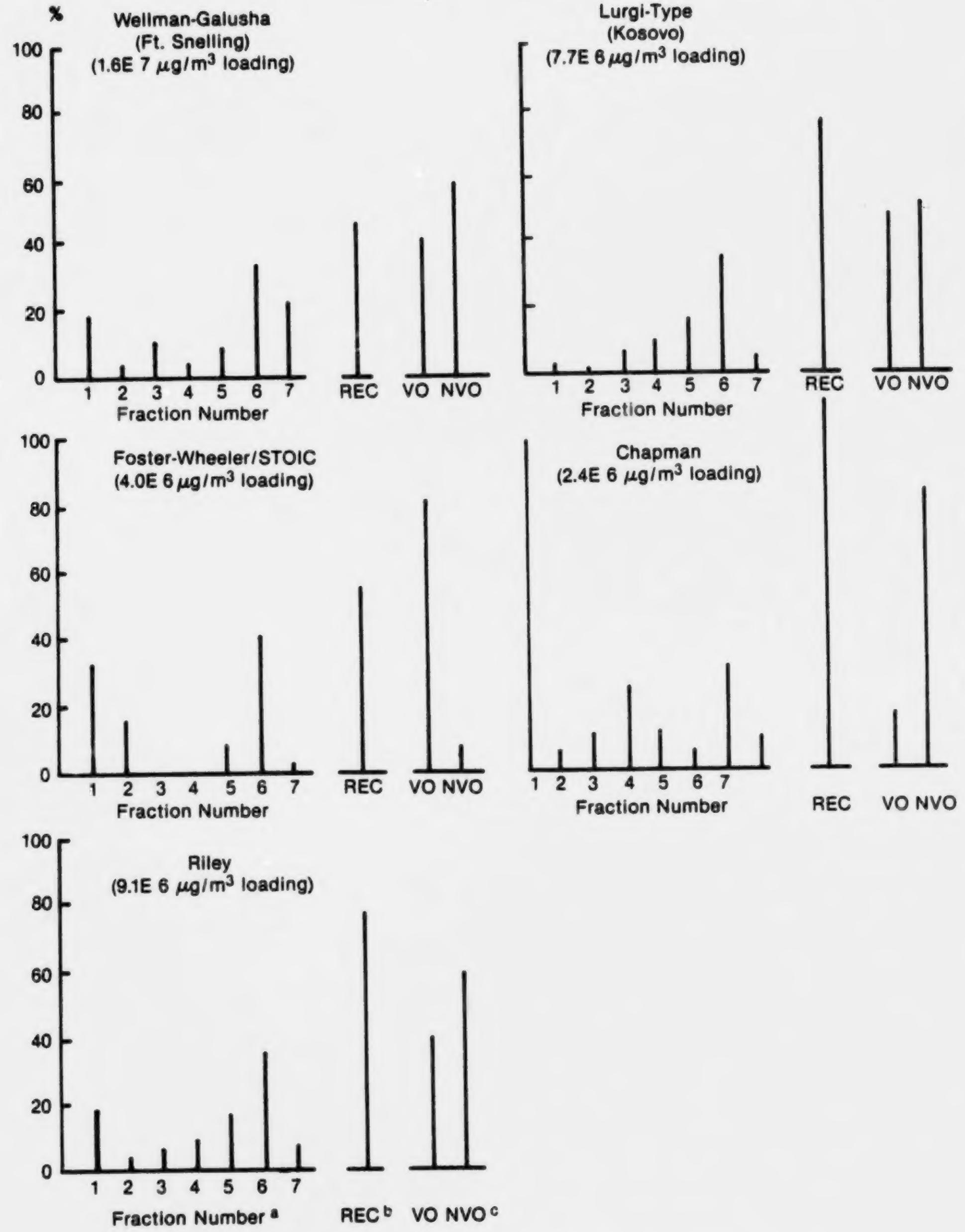
Except for the Glen Gery case, this comparison indicates that there is little difference between these gasifiers in their ogranics production while operated on coals with similar volatile content. There is no significant difference in distribution of the light hydrocarbons among these product gases. The reason for the Glen Gery difference is the use of low volatile anthracite.

More detailed information about characteristics of the organics in these product gas streams is provided by the fractionation results summarized in Figure 19 which shows:



[a] Percent volatile in feed coal.
[b] Benzene, Toluene, Xylene included.
[c] Pentanes and hexanes not determined.

Figure 18. Summary of light hydrocarbons in product gas.



[a] Percent of eluted in each LC fraction.
[b] Percent recovered from LC.
[c] Percent volatile and percent non-volatile organics.

Figure 19. Comparison of organics in product gas.

- Organic loading in ug/m^3,
- % volatile organics (TCO) and % non-volatile organics (GRAV),
- % recovered from column chromatography (REC), and
- % of eluted quantity found in each LC fraction.

The following example illustrates the quantitative use of Figure 19. The data from the Wellman-Galusha gasifier at Fort Snelling show 58% non-volatile organics indicating that the GRAV determination found 8.7E 6 ug/m^3 (58% of the total loading shown) of organics greater than C_{12} in the aerosols and vapors transported by the gas stream. When separated by column chromatography into 7 fractions, nineteen percent of the eluted organics were found in fraction 1 that should contain non-polar substances such as hydrocarbons while thirty-three percent of the eluted organics was found in fraction 6 that contains polar substances such as phenols. However, the figure shows that only 46% of the organics loaded on the column were recovered. Therefore, the concentration of fraction 6 is: 0.3 x 0.46 x 1.5E 7 = 2.5E 6 ug/m^3 representing about 17% of the total organics. By comparing the respective bar graphs for each process several observations can be made:

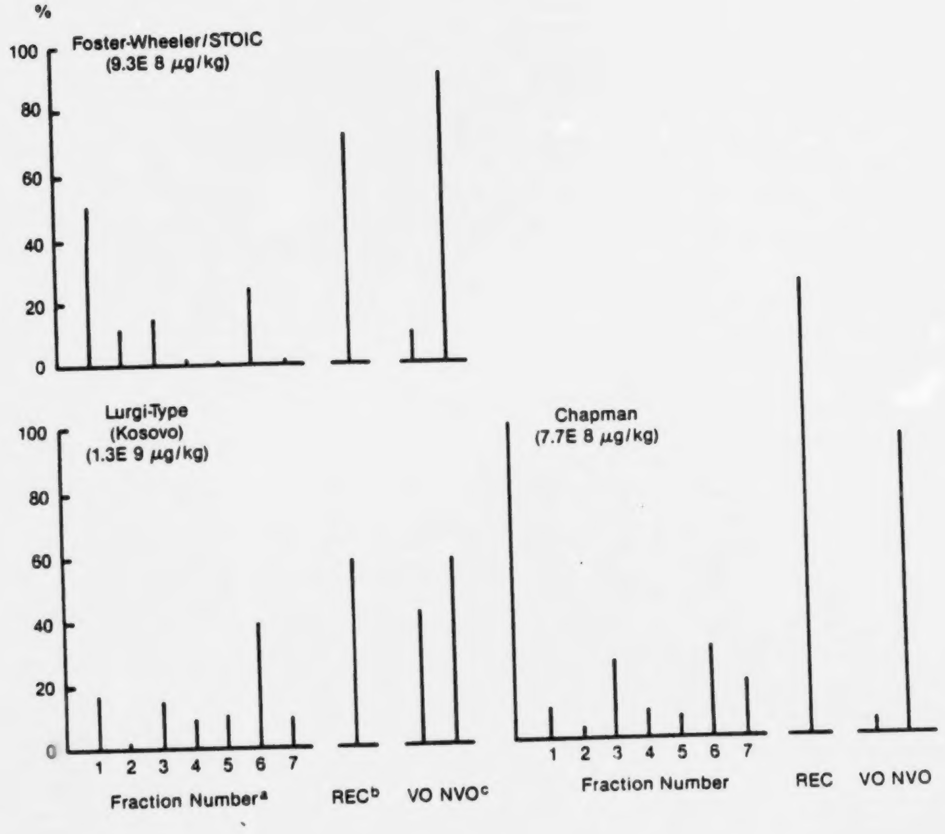
- Organics from all processes show similar distributions with respect to polar components as indicated by fraction 6.
- Three processes; Wellman-Galusha (Ft. Snelling), Foster-Wheeler/STOIC, and Riley, show significant quantities of non-polar hydrocarbons while Chapman and the Lurgi-type facility at Kosovo do not. Because the Kosovo process is known to produce large quantities of light and intermediate organics, the low quantities reflected in Figure 19 are suspect and may be attributed to the analyses.
- Recoveries from LC were generally adequate with a mean value of 77% ± 27%.

- The distribution between volatiles (total chromatographable organics) and non-volatiles (gravimetrically determined organics) varies among the respective processes. The greatest difference is shown between the Foster-Wheeler/STOIC and the Chapman gasifier. Only small differences in the VO/NVO distributions exist among the other three processes.

The difference between the VO/NVO distribution of the Foster-Wheeler/STOIC and Chapman gasifiers is partially indicative of the difference in sampling points. The combined gas from the Foster-Wheeler/STOIC gasifier has a significant portion of the oil and tar aerosols removed from the dirty top gas by an ESP prior to being combined with the bottom gas that is comparatively organic free. In contrast, the gas from the Chapman gasifier came directly through the coal devolatilization zone. Although both tar/oils show about 5% as VO and about 95% as NVO, their LC profiles from the tar/oil screening analyses differ as shown in Figure 20. The STOIC ESP oil shows a large non-polar content similar to the organics collected from that product gas whereas the Chapman tar shows a broad distribution like the condensables collected from that coal feeder vent gas. In contrast to the Chapman similarities, the LC profile of the Kosovo tar (Figure 20) does not match that of the condensable organics in the gas escaping from the low pressure coal lock vent (Figure 19); the tar shows a greater content of non-polar hydrocarbons than do the condensable organics. Overall the VO/NVO distributions and the LC recoveries are about the same in both Kosovo samples.

Organic Loadings in Solid-Phase Streams

The organic loadings and LC distributions of organics in gasifier ash from each of three processes (Wellman-Galusha at Ft. Snelling, Foster-Wheeler/STOIC, and Riley), are shown in Figure 21. Kosovo ash, not included in the figure, had a loading of 4.0E 5 mg/kg that was 100% NVO, and was unfractionated. The organic loading of the Foster-Wheeler/STOIC ash is three orders of magnitude lower than the other ashes and shows a high volatile organic content compared to the ash from the other sources. Whether the difference is real

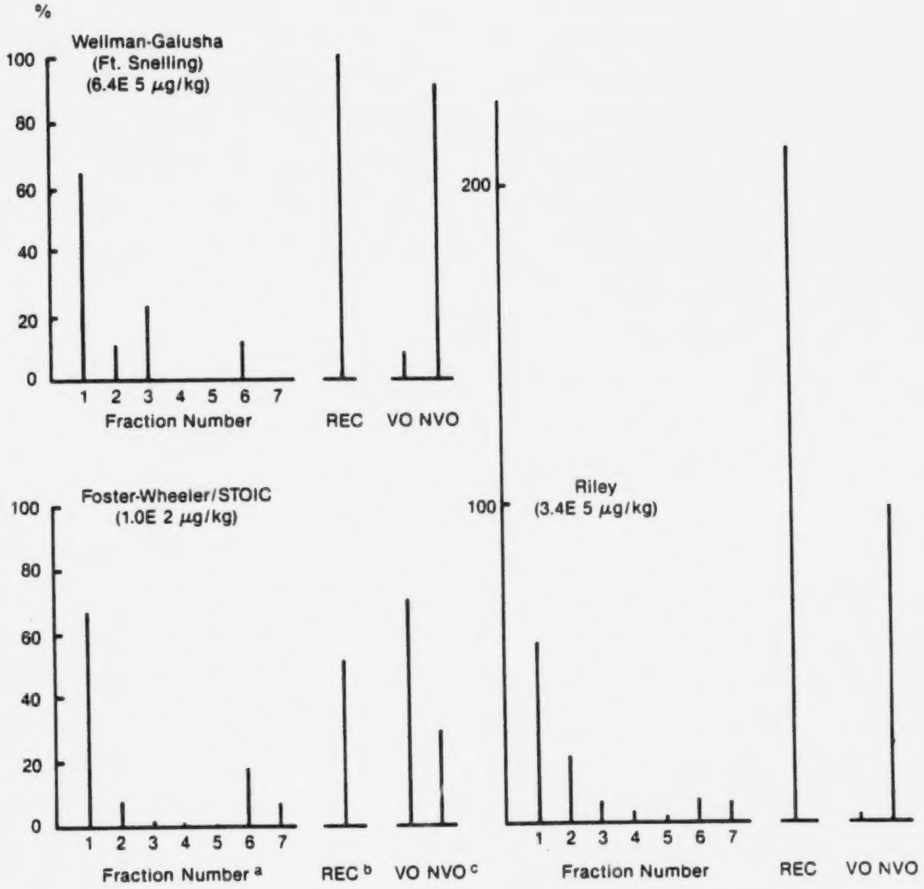


[a] Percent of eluted in each LC fraction.

[b] Percent recovered fromLC (Rec).

[c] Percent volatile (VO) and percent non-volatile (NVO) organics.

Figure 20. Comparison of tar/oil from different gasifiers.



[a] Percent eluted in each fraction.
[b] Percent recovered (REC) from LC.
[c] Percent volatile (VO) and percent non-volatile (NVO) organics in extract.

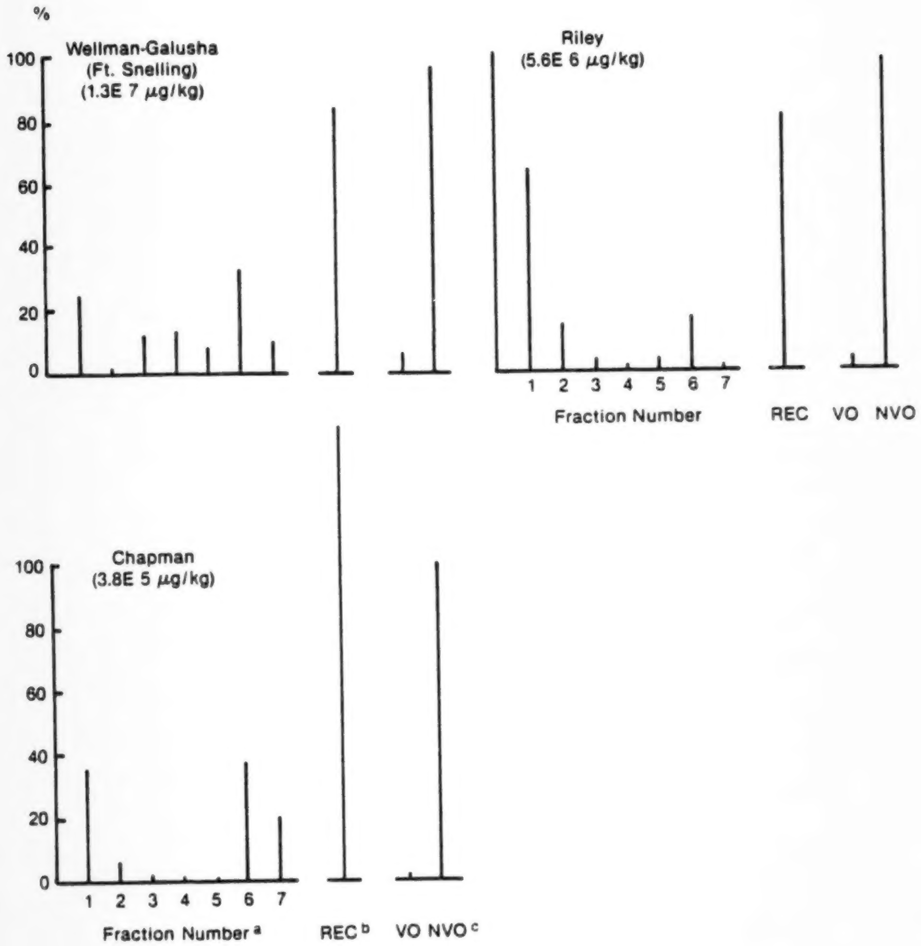
Figure 21. Comparison of organics from gasifier ash.

cannot be ascertained from the data available. The greater than 200% recovery from the LC of the Riley ash-organics indicates either error inherent in calculating a small aliquot back to the source, or contamination of that sample, or both. In spite of uncertainties in the overall recoveries, the LC profiles of the organics from these three ashes are remarkably similar and show a high level of non-volatile non-polar organics (e.g., straight chain paraffins or more likely, long-chain carboxylic acids in which the carboxylic acid moiety is masked by the long paraffinic chain).

The organic loadings and LC distributions in the cyclone dust from the Wellman-Galusha (Ft. Snelling), Riley, and Chapman gasifiers are shown in Figure 22. The organic loading of the Chapman cyclone dust is an order of magnitude lower than the Riley and the Wellman-Galusha (Ft. Snelling) dusts. The difference is not unreasonable when the difference in the particle geometry is considered. The cyclone dust from the Chapman gasifier consists of hollow spheres or broken sphere segments produced by coal swelling in free fall. Such low surface area particles tend to have lower carrying capacity than the smaller aggregate dust-like particles produced in the other gasifiers (1). Although the VO/NVO ratios are similar in all samples, the LC distribution indicates differences in organic distribution; the Ft. Snelling sample contains a quantity of moderately polar material (fractions 3-5) not found in the others while the Riley sample shows a greater amount of non-polar (fractions 1-2) organics.

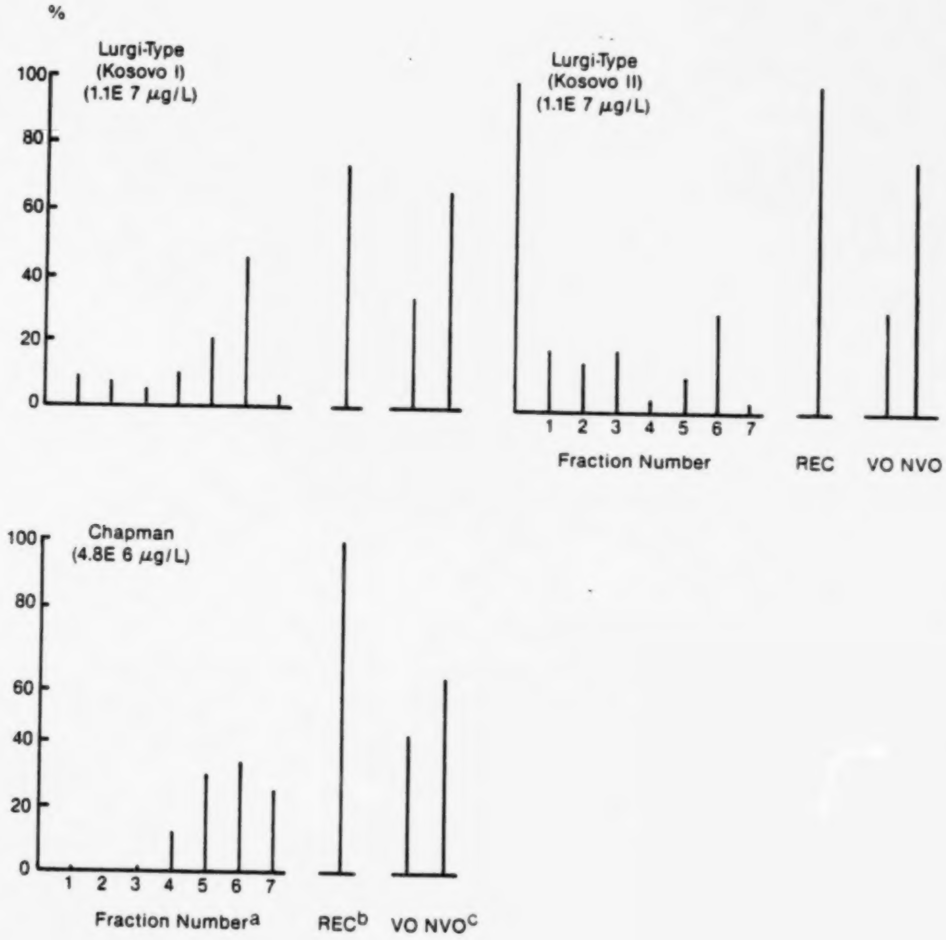
Organic Loadings in Aqueous Streams

The loadings and the LC distribution of organics extracted from product gas liquor from two sources are shown in Figure 23. The LC profile of Kosovo samples shows more non-polar material than the Chapman sample but samples from both gasifiers show a large amount of material attributable to phenols. However, Kosovo sample II shows nearly an equal balance of polar and non-polar material. Both Kosovo samples show an organic loading of 1.1E7 ug/L while the Chapman sample shows a loading of 4.8E 6 ug/L (2). However, the Chapman liquor, sampled during a later study (4), showed a loading similar to Kosovo liquor as is shown below.



[a] Percent eluted in each fraction.
[b] Percent recovered (REC) from LC.
[c] Percent volatile (VO) and Percent non-volatile (NVO) organics in extract.

Figure 22. Comparison of organics extracted from cyclone dust.



[a] Percent eluted in each fraction.
[b] Percent recovered (REC) from LC.
[c] Percent volatile (VO) and percent non-volatile (NVO) in extract.

Figure 23. Comparison of organics extracted from gas liquor.

Chapman Gas Liquor	ug/L	% VO	% NVO
Acid Extractable Compounds	7.9E6	32	68
Base/Neutral Extractable Compounds	1.4E6	74	26
Total Organics	9.3E6	38	62

The organic loading of this sample of Chapman liquor was 9.3E 6 ug/L which is comparable to the Kosovo loading. Although the Chapman gas liquor is recirculated, it appears from these results that its organic loading is not constant but varies with plant operation. Among the factors which may influence organic loading are coal moisture and frequency of blow-down to the evaporator. The extraction data above show that 58% (0.68 x 7900 = 5300 mg/L or 58%) of these extractable organics are acid extractable NVOs, most likely phenolic compounds.

The water quality parameters pertaining to organics from several aqueous streams and leachates are listed in Table 6. A summary of these data indicates that:

- Gasifier ash quench water is comparatively organic free.

- Settler underflow from the Texaco gasifier contains significantly more organic carbon than ash quench water.

- Cyclone dust quench water from the Wellman-Galusha (Ft. Snelling) gasifier contains more TOC (185 mg/L) than that gasifier ash quench water (16 mg/L). The cyclone dust quench water TOC concentration is about the same as in Texaco settler underflow (195 mg/L), which is an analogous process stream.

- Gas liquor from the Chapman and the Lurgi-type (Kosovo) gasifiers is high in all categories of organic water quality parameters. It can be noted also, that:

  -- There is no apparent correlation between the COD and the TOC values;

TABLE 6. SELECTED WATER QUALITY PARAMETERS AND TOTAL ORGANICS (TO) IN AQUEOUS STREAMS AND SOLID-PHASE STREAM LEACHATES FROM VARIOUS PROCESSES

Process	Stream	mg/L TOC	Phenol	COD	Dissolved BOD	Oil & Grease	TO	%NVO
Wellman-Galusha (Fort Snelling)	Gasifier Ash Sluice Water	16	0.36	0.76	28-64	NA[a]	125	90
Foster-Wheeler/STOIC	Gasifier Ash Sluice Water	3.2	0.006	100 ±17	<1-28	NA	NA	NA
Riley	Gasifier Ash Sluice Water	NA	NA	NA	NA	NA	11.5	64
Lurgi-Type (Kosovo)	Gasifier Ash Sluice Water	NA	0.17	1.460	90	ND	NA	NA
Chapman	Gasifier Ash Sluice Water	0.3	NA	NA	NA	NA	NA[b]	NA[b]
Wellman-Galusha (Glen Gery)	Gasifier Ash Sluice Water	140	ND[c]	20	40	NA	46	14
Texaco (Ruhrkohle)	Settler Underflow	195 ± 100	<0.018	177 ± 29	315	3	NA	NA
Koppers-Totzek (Modderfontein)	Settler Underflow	5.3	0.104	4	4	NA	0.6	<15
Wellman-Galusha (Fort Snelling	Gasifier Ash Leachate	<1	0.002	1,710	2,970	NA	NA	NA
Wellman-Galusha (Fort Snelling)	Cyclone Dust Quench Water	185	9.8	800	62-85	NA	60	94
Wellman-Galusha (Fort Snelling)	Cyclone Dust Leachate	<1	0.38	1,410	3,150	NA	NA	NA
Chapman	Phenosolvan Inlet	4,970	2,120	18,900	9,030	400	11,000	67
Chapman[b]	Separator Liquor	NA	NA	NA	NA	NA	9200	6200
Lurgi-Type (Kosovo)	Separator Liquor	NA	NA	22,000	6,530	NA	4,800	55
Lurgi-Type (Kosovo)	Phenosolvan Outlet	1,470	230	7,910	2,350	200	NA	NA
Koppers-Totzek (Modderfontein)	Compressor Condensate	140	0.01	600	550	NA	4	>90
Koppers-Totzek (Modderfontein)	Rectisol Condensate	15	0.01	350	120	NA	12	>90
KRW	Quench[d]	80	6	270	NA	14	NA	NA
KRW	Recycle Cooler	30	3	160	NA	4	NA	NA
KRW	Separator Pit	50	0.02	180	NA	4	NA	NA
KRW	Makeup	40	0.02	130	NA	3	NA	NA

The following were sampled at a different time for a separate study (15):

Process	Stream	TOC	Phenol	COD	Dissolved BOD	Oil & Grease	TO	%NVO
Chapman	Separator Liquor	9,430	2,130	28,500	15,900	540	NA	NA
Chapman	Extracted Liquor (Laboratory)	3,290	3.0	15,500	2,800	<10	NA	NA
Chapman	Acidified Extraction	1,830	NA	7,230	NA	NA	NA	NA
Lurgi-Type (Kosovo)	Separator Liquor	6,490	3,030	20,200	13,200	917	NA	NA
	Extracted Liquor	2,010	9	4,940	3,080	<10	NA	NA
	Acidified Liquor	1,894	NA	4,270	NA	NA	NA	NA
Coke Oven[e]	Condensate	3,420	1,140	4,860	3,420	700	NA	NA
	Extracted Condensate	602	9	2,770	727	<10	NA	NA

---

[a] NA = Not analyzed.
[b] Listed in ref. 2 as 0 mg/L; no detection limit indicated.
[c] ND = <0.7 ug/L.
[d] The KRW values are average values for two different fuels. See discussion in text.
[e] Coke oven gas liquor was included for reference to a destructive distillation process.

-- There is no apparent correlation between TOC and TO;

-- There is no apparent correlation between COD and TO.

Consequently, no one method used to determine organics in water appears to be a reliable surrogate for the others.

The coal gasification plant at the former Grand Forks Energy and Technology Center (GFETC) of the U.S. Department of Energy has been reported to produce large amounts of hydantoins in the aqueous condensate (19). It was suggested that these compounds may arise from the reaction of ketones or aldehydes with ammonia, carbonate, and cyanide. The major portion of the refractory organics in that condensate was attributed to 5,5'-dimethyl hydantoin (5,5'-DMH) which was found at levels ranging from 300 to 2000 mg/L. Since hydantoins had not been identified at the Kosovo facility or analyzed in other studies, a specific effort was made to determine the level of hydantoins in the Kosovo wastewater. The findings are summarized below:

Hydantoin	Kosovo (mg/L)	Grand Forks (mg/L)
5,5'-DMH	2	650
5-ethyl-5-methyl hydantoin	0.6	280

This finding was supported by infrared spectra which clearly showed evidence of alkyl hydantoins in GFETC water and not in the Kosovo wastewater. This seems to indicate that the GFETC fixed-bed slagging gasifier produces different refractory organics than the lower temperature dry bottom Lurgi-type gasifier at Kosovo.

DETAILED ORGANIC ANALYSES

A variety of methods have been used to characterize organics in the discharges from coal gasification plants. The results have ranged from functional group identification by infrared spectrometry to complete speciation of chromatographable components by GC-mass spectrometry. For detailed organic analyses, samples generally were separated into acid and base-neutral fractions prior to analysis and speciation by GC-MS. Methods have included the following:

- GC-MS,
- Capillary GC-MS,
- Low Resolution Mass Spectrometry (LRMS),
- Selective Detection (S, N, Cl) GC, and
- Infrared Spectrophotometry (IR).

The data presented in this section have been selected to illustrate the composition and complexity of the mixtures of organics associated with these gasification processes and also to indicate the extent to which the speciated organics account for the total organics in the various streams. Additional supporting data are included in Appendix C.

Organics from the Chapman Gasifier

Of the sources for this report, the Chapman gasifier study provided the most thorough speciation of organics. Streams selected for detailed analyses at this facility were:

- Coal Feeder Vent,
- Separator Vent,
- Separator Liquor,
- Separator Tar,
- Gasifier Ash, and
- Cyclone Dust.

Samples were separated into acid and base-neutral fractions prior to analyses by GC-MS. A total of 111 compounds from 14 different classes of organics were identified and quantified in samples from six streams (Table 7) of the

TABLE 7. ORGANIC SPECIES FROM THE CHAPMAN GASIFIER

SPECIATION[a]	COAL FEEDER ($\mu g/m^3$)	SEPARATOR VENT ($\mu g/m^3$)	SEPARATOR LIQUOR ($\mu g/L$)	TAR ($\mu g/m^3$)	GASIFIER ASH ($\mu g/g$)	CYCLONE DUST ($\mu g/g$)
Total Organics	7.8E5	4.2E6	4.8E6	7.7E5		
% VO	42	45	42	5		
% NVO	58	55	58	95		
$\geq C_6$ Alkanes	2E2	2E3	2E2	1E1	3E1	
$\geq C_{13}$ Alkanes	3E3			2E2		
Methylanisole		3E3				
$>C_6$ Aliphatic Alcohols	2E2	2E1	2E2	4E2		
$>C_{13}$ Aliphatic Alcohols	2E1		1E4			
Methylacetophenone		2E1				
Phthalic Acid	1E2		1E4	2E2	3E0	
Phthalates	7E2	2E3	7E2	6E3		8E2
Adipates		9E3	6E2	5E3	4E2	6E2
$>C_9$ Aliphatic Esters				3E1		
Benzonitrile		1E2				
Cyanotoluene		1E1				
Pyrrolidine	6E1					
Aminonaphthalene/Methylquinoline	1E2	3E3	9E1			
Methylaminonaphthalene/C_2-Alkylquinoline	2E2	2E2				
Aniline		1E2	3E2			
C_1-Alkylaniline		4E2				
Aminonaphthalene/Methylquinoline		3E3	9E1	1E2		
Methylaminonaphthalene/C_2-Alkylquinoline		2E2		1E2		
C_2-Alkylaminonaphthalene/ C_3-Alkylquinoline		6E1		3E1		
Aminotoluene/C_2-Alkylpyridine			4E2			
C_2-Alkylaniline/C_3-Alkylpyridine			1E2	1E0		
Methylpyrrolene			6E1			
Methylaminoindane			8E1			
Methylaminoindene			2E2			
C_3-Alkylaniline/C_4-Alkylpyridine				1E1		
Aminotetralin/Methylaminoindane				6E2		
Aminoacenaphthylene/Carbazole				1E1		
Methylaminoacenaphthylene/Aminofluorene/				2E1		
Aminopyrene/Aminofluoranthene				2E1		
Benzoaminofluorene				1E1		
Methylbenzoaminofluorene				5E0		
C_2-Alkylbenzene	2E3	3E2			1E1	
C_3-Alkylbenzene	7E2	7E2				
Styrene	2E2					
Indan/C_3-Alkenylbenzene	2E3	2E3				
Tetrahydronaphthalene	1E3					
Methyl Indan	2E2					
Dihydronaphthalene/Methyl Indene	1E3	5E3		1E2		
Phenylacetylene		2E2				
Methyldihydronaphthalene/C_2-Alkylindene		3E3		1E2		

(Continued)

TABLE 7. (Continued)

SPECIATION[a]	COAL FEEDER ($\mu g/m^3$)	SEPARATOR VENT ($\mu g/m^3$)	SEPARATOR LIQUOR ($\mu g/L$)	TAR ($\mu g/m^3$)	GASIFIER ASH ($\mu g/g$)	CYCLONE DUST ($\mu g/g$)
C_2-Alkyldihydronaphthalene/ C_3-Alkylindene		1E3				
Tetrahydronaphthalene/Methylindan		7E2				
Methyltetrahydronaphthalene/ C_2-Alkylindan		3E3				
C_2-Alkyltetrahydronaphthalene/ C_3-Alkylindan		4E3				
Biphenyl/Acenaphthene		9E3		6E2		
Methylbiphenyl/Methylacenaphthene		4E3		1E2		
C_2-Alkylbiphenyl/C_2-Alkylacenaphthene		6E2		4E2		
C_3-Alkylbiphenyl/C_3-Alkylacenaphthene		8E2		3E2		
Phenol	3E2	3E5		4E2		
C_1 Alkyl Phenol	8E2	5E5		2E3		
C_2 Alkyl Phenol	8E2	7E5		1E3		
C_3 Alkyl Phenol	1E2	2E4		1E2		
C_4 Alkyl Phenol	9E0	8E2				
Indenol	1E2			1E2		
Indanol	1E2			1E1		
Naphthol	2E2			4E2		
Methylnaphthol	3E2			4E2		
C_2-Alkylnaphthol	2E1			5E1		
Hydroxyacenaphthylene	3E1			6E1		
Phenylphenol/Acenaphthol	5E1			2E1		
Methylphenylphenol/Methylacenaphthol	7E1					
C_2-Alkylphenylphenol/C_2-Alkylacenaphthol	1E2			2E2		
C_3-Alkylphenylphenol/C_3-Alkylacenaphthol	6E1			4E1		
Hydroxyphenanthrene/Hydroxyanthracene	3E1			2E2		
Dihydroxybenzene			1E4			
Methyldihydroxybenzene			2E3			
Methylhydroxyacenaphthylene/Fluorenol				1E1		
C_5-Alkylhydroxyanthracene/C_5-Alkyl- hydroxyphenanthrene				6E1		
C_3-Alkylhydroxypyrene/C_3-Alkyl- hydroxyfluoranthene				1E2		
Hydroxybenzofluorene				2E2		
Naphthalene	1E4	5E3	8E2		2E1	5E2
Methylnaphthalene	1E4	2E4	4E2	1E3	4E1	
C_2-Alkylnaphthalene	2E3	7E3	1E2			
Methylacenaphthene/Dibenzofuran/ Methylbiphenyl	8E2					
C_2-Alkylacenaphthene/Methyldibenzofuran/ C_2-Alkylbiphenyl	4E2			1E3		
Acenaphthylene	5E3	3E3	4E2	2E3		
Methylacenaphthylene/Fluorene	2E4	1E3		2E3		
C_2-Alkylacenaphthylene/Methylfluorene	1E3	6E2		1E3		
Phenanthrene/Anthracene	3E3	1E3		2E3		
Methylphenanthrene	2E3	1E2		1E3		
Benz(a)anthracene (<5 isomers)	1E3			6E2		
Benzo(a)pyrene ($\leq$6 isomers)	8E2					
Benzoperylene	3E2		9E2	1E2		
C_2-Alkylphenanthrene/C_2-Alkylanthracene				2E2		
Methylbenzophenanthrene ($\leq$5 isomers)				6E2		

(Continued)

TABLE 7. (Continued)

SPECIATION[a]	COAL FEEDER ($\mu g/m^3$)	SEPARATOR VENT ($\mu g/m^3$)	SEPARATOR LIQUOR ($\mu g/L$)	TAR ($\mu g/m^3$)	GASIFIER ASH ($\mu g/g$)	CYCLONE DUST ($\mu g/g$)
Indene		4E3	8E2	3E2		
Fluoranthene/Pyrene				1E3		
Benzofluorene/Methylpyrene				2E3		
Quinoline	5E1	2E2	2E2	4E2		
Methylquinoline/Aminonaphthalene	1E2	3E3	9E1	1E2		
C_2-Alkylquinoline/Methylaminonaphthalene	2E2	2E2		1E2		
Carbazole	5E1			2E1		
Acridine/Benzoquinoline/Phenanthridine	2E2			2E1		
Methylacridine/Methylbenzoquinoline/ Methylphenanthridine	1E2			6E1		
Benzoacridine/Dibenzoquinoline/ Benzophenanthridine	8E1					
Methylbenzoacridine/Methyldibenzoquinoline/ Methylbenzophenanthridine	6E1					
C_3-Alkylpyrrole			1E2			
Indole			2E3			
Methylindole			4E2			
Methylcarbazole/Aminofluorene/ Methylaminoacenaphthylene				2E1		
C_2-Alkylacridine/C_2-Alkylbenzoquinoline				2E1		
C_3-Alkylacridine/C_3-Alkylbenzoquinoline				5E0		
Pyridine		2E2				
Picoline/Anilene		6E2	3E2			
C_2-Alkylpyridine/Aminotoluene		2E3	4E2			
C_3-Alkylpyridine/C_2-Alkylaniline		1E3	1E2	1E0		
C_4-Alkylpyridine		2E2		1E1		
C_3-Alkylquinoline/C_3-Alkylamino- naphthalene		6E1		3E1		
Dibenzofuran				4E2		
Benzothiophene		2E2				
Specific Organics Subtotal	7.2E4	1.6E6	2.0E6	3.6E4	4.0E0	1.3E1
Number of Components Detected	53	53	37	91	6	2
% of Total Organics	9.2	38	42	5		

[a] Grouping is based on Table A-5 of Ref. 8.

Chapman gasifier. Many of the compounds identified have isomeric structures so that the actual number of components contained by these streams might be much larger than the number given. It is anticipated that the tar contains many more components than those found by GC-MS. Although the discharge from the coal feeder vent contains raw product gas, it does not reveal all of the components occurring in the hot product gas that transports the tar.

It can be assumed that all of the components found are produced in the gasifier. Some components (e.g., naphthalenes, phenols, and nitrogen heterocyclics) are found in all four organic-bearing streams: coal feeder vent, separator vent, separator liquor, and tar. Many components found in the separator liquor and separator vent gas were not found in the coal feeder vent gas even though these components must have originated in the gasifier and were transported in the hot crude product gas. There are two plausible explanations for their not being found in the coal feeder vent gas.

- The coal feeder vent gas was cooler than the crude product gas and, therefore, did not transport many of the higher boiling components.
- The liquor and tar accumulate and concentrate many components which are below the threshold of detectability in the vent gases.

From the data in Table 7, it can be seen that:

- Gasifier ash and cyclone dust are essentially free of organics;
- Only a limited number of components are common to all organicbearing streams; and
- Considerable fractionation occurs between the tar, liquor, and vent gas in the separator; these streams show few common species.

As shown in Table 8, the identified species account for only a portion of the total organics. Accountability varies from about 50% in the liquor to about 10% for the coal feeder vent gas and about 5% for the tar. These results are from two independent samples, but levels and general compositions are sufficiently uniform to allow this comparison.

Two values are reported for total organics by GC-MS in Table 8. One value is taken from Table 5-7 of Reference 2, the other value was obtained by summing the individual values listed in Table 7. It is not known whether the difference between the two values is the result of summing rounded-off values or whether the values presented in the reference were obtained by a separate analysis. Regardless of this apparent difference, the indications of the two data columns are the same: the species determined probably account for less than half of the organics present, and only a small portion of the components in gasifier tar have been identified and quantified.

Inspection of the data in Table 7 indicates that a few components in each stream make up a majority of the identified mass. This observation is illustrated by Table 9 where the major components of the organic-bearing streams of the Chapman gasifier are defined. The summary shows that three components comprise 53% of the condensable organics in the coal feeder vent gas, three other components comprise greater than 90% of the identified organics from the separator liquor and the separator vent gas, and six components (four in common with other streams) comprise greater than 50% of the identified organics in tar. From the data in Table 9, it is evident that the identified species provide a reasonable indication of the composition of the organics in the separator liquor and separator vent gas where a few dominant species comprise about 40% of the mass. But the identified species do not provide as complete a description of the composition of those organics in the separator tar nor in the tar-bearing coal feeder vent gas where only 10% of the mass has been speciated and about 5% of the mass is represented by identified major components.

TABLE 8. CHAPMAN GASIFIER: ACCOUNTING OF TOTAL ORGANICS BY GC-MS AND BY SUMMING SPECIES RELATIVE TO TOTAL ORGANICS BY SCREENING

		Total Organics			
Stream	Total Organics by Screening	Estimated by GC-MS[a]	Percent Recovered[b]	Sum of Components in Table 7	Percent Recovered[b]
Coal Feeder Vent (ug/m^3)	7.8E5	1.0E5	13	7.2E4	9.2
Separator Discharge Vent (ug/m^3)	4.2E6	1.7E6	40	1.6E6	38
Separator Liquor (ug/g)	4.8E6	2.4E6	50	2.0E6	42
Separator Tar (ug/g)	7.7E5	5.1E4	6.6	3.6E4	4.7

[a] Values from Table 5-7 ref. 2.
[b] Percent relative to TO by screening.

TABLE 9. CHAPMAN GASIFIER - MAJOR COMPONENT SUMMARY[a]

	Coal Feeder Vent Gas (ug/m^3)	Separator Vent Gas (ug/m^3)	Separator Liquor (ug/L)	Tar (ug/m^3)
Total Organics by Screening	7.8E5	4.2E6	4.8E6	7.7E5
Estimated by GC-MS	1.0E5	1.7E6	2.4E6	5.1E4
Sum identified (Table 7)	7.2E4	1.6E6	2.0E6	3.6E4
Percent Recovered	13-9	40-38	50-42	7-5
Major Components:				
Naphthalene	1E4			
Methylnaphthalene	1E4			
Acenaphthalene				2E3
Methyl acenaphthalene	2E4			2E3
Phenanthrene/anthracene				2E3
Benzofluorene/methyl pyrene				2E3
Phenol		3E5	6E5	
C_1-Alkyl phenol		5E5	1E6	2E3
C_2-Alkyl phenols		7E5	3E5	4E3
Sum of Major Components	4.0E4	1.5E6	1.9E6	1.4E4
Sum of Stream Components	7.2E4	1.6E6	2.0E6	2.5E4 [b]
Major Components as % of Sum of Stream Components	56	94	95	56
Total Number Determined	53	53	37	71
% Speciated relative to TO	11	39	46	6
% Major Components relative to TCO	6	37	44	3

[a] Components greater than 10% of total.

[b] Artifacts of sampling and sample handling (plasticizers) were subtracted from total to obtain values reported here.

This detailed analysis was not intended to speciate the bulk compositions of these materials but rather to identify potentially hazardous compounds within twenty-six organic classes and then to assess the potential for environmental burden from these substances. The quantifications were estimates and should not be used as a quantitative statement of composition. The arithmetical treatment of the percentages shown above is to stimulate an awareness of the limitations of these data rather than to provide a definitive statement of composition for the organics in these streams.

Organics from the Foster-Wheeler/STOIC Gasifier

The organics from the several streams of the Foster-Wheeler/STOIC gasifier were analyzed by GC-MS. The separations were made on a high resolution, 100m quartz capillary GC column using the same conditions for each stream. While some peaks in these chromatograms were readily identifiable, many others were not. Therefore, many peaks are not identified specifically. Since each peak of a gas chromatogram represents at least one component and no component can produce two peaks, the number of peaks on each chromatogram indicates a minimum number of components contained by each sample. Since elution was generally in the order of increasing boiling point in this case, the retention times provide a probable boiling point for each component.

An internal standard (d_{10}-anthracene) was used with all samples to permit peak areas to be converted to mass units relative to the internal standard so that each component could be quantified. The results of these detailed analyses are shown in Appendix C (Table C-4) and summarized in Table 10.

The speciation data summarized were compiled from seven different streams and sequenced by chromatograph retention time (Table C-4). Therefore, it is possible to compare streams even though a given component may be entered at more than one retention time and different unidentified components may be entered at the same retention time. Several observations can be made with regard to these data.

TABLE 10. FOSTER-WHEELER/STOIC GASIFIER - SUMMARY OF DETAILED ORGANIC ANALYSES

	Product Gas	ESP Oil	Gasifier Ash	Cyclone Dust	Ash Pan Water	Product Gas Combustion Emissions	ESP Oil Combustion Emissions	Mean and S.D.
Reference Table[a]	B57	B58	B52	B54	B53	B56	B55	-
Units of Concentration	ug/m^3	ug/g	ug/g	ug/g	ug/L	ug/m^3	ug/m^3	%
Total Organics Concentration	4.0E6	9.3E5	1.0E2	1.2E2	1.0E3	2.7E1	2.7E3	-
Organic Concentration per GC-MS	5.1E5	9.4E4	1.9E1	1.3E1	1.9E2	1.5E2	4.5E2	-
Concentration of Identified Components	3.7E5	7.3E4	1.5E1	4.6E0	1.4E2	1.1E2	4.4E2	-
% of Total Organics Eluted	13	10	19	11	19	550	17	-
% of Eluted Organics Identified	73	78	72	34	68	74	98	-
% of Total Organics Identified	9	8	14	4	13	400[b]	17	11 ±5
Number of Components Eluting	134	139	108	51	31	32	26	-
Number Not Identified (NI)	51	79	52	33	21	18	2	-
% Identified (Partially)	62	43	52	35	32	44	92	51 ±20
Initial Boiling Point °C[c]	150	200	150	70	160	165	155	-
Final Boiling Point °C	400	460	410	450	440	400	420	-

[a] Reference 11.
[b] Value excluded from mean.
[c] Based on chromatographic retention.
(-) No entry

- About half (51 ± 20%) of the components eluting from the GC column have been identified by compound class or component type.

- The partially identified components account for about 70% (71 ± 19%) of the eluting mass.

- This identified mass accounts for only about 10% of total organics as determined by the Level I screening (TCO + GRAV).

- The product gas combustion emission presents an anomaly in that the mass of the determined species exceeds the mass of the total organics. This value was therefore excluded from the averages in the table.

- The boiling points of the determined species range between about 150°C and 400°C (estimated from the retention of normal paraffins).

- Identified compounds may be grouped into the following classifications:

  -- Paraffins and Olefins:
  Straight chain paraffins, C_{10}-C_{29}
  Branched and cyclo-paraffins
  Olefins

  -- Phenols:
  Phenol and alkyl phenols
  Alkyl polyhydroxybenzenes

  -- Aromatics and Polyaromatics:
  Alkyl benzenes and naphthalenes
  Indans and alkyl indans
  Biphenyls
  Hydronaphthalenes and alkyl hydronaphthalenes

- Aldehydes:
  - Benzaldehyde

- Esters:
  - Methyl benzoate
  - Phthalates, possibly process originated
  - Plasticizers: phthalates and adipates not originating in the gasifier.

- Halogenated Compounds:
  - Trichloropropane and other chloroalkanes
  - Dichlorophenol

- Sulfur (S_8)

Several specific observations can be made about composition of the organics in the respective streams listed in Table C-5 (appendix) and summarized in Table 10.

> Combined Product Gas - Ten components which make up 24% of the relative response of the eluting mass of organics from the combined product gas are phenol, cresol, an alkyl benzene, a methyl indane, plus several alkyl naphthalenes. Cresol, present at 4% of relative mass, is the largest component.
>
> ESP Oil - Normal hydrocarbons ranging from C_{19}-C_{29} make up 39% of the response of the eluting mass. C_{25}, present at about 6%, is the largest component. A non-paraffinic component (retention time of 39.40 min), present at 5%, is not identified. The concentrations of a list of aminoaromatic compounds presented in Appendix C Table C-5 are from an independent analysis of ESP oil (14).
>
> Gasifier Ash - The major organic components in the gasifier ash are C_{10}-C_{14} normal hydrocarbons (about 31%). An unidentified component

(retention time of 22.33 min) is present at 6% which is at about the same level as the major paraffins; C_{10}, C_{11} and C_{14}, each comprise more than 5% of the speciated organics (see Appendix C Table 5).

Cyclone Dust - Three unidentified major components make up about 40% of the organics. The major component (retention time of 3.51 min) is comparatively low boiling (<100°C) and makes up about 25% of the eluting mass. (This material may have originated from the extracting solvent, methylene chloride, since the component eluting immediately after it is also a chlorine-containing component). These organics contain about 20% long chain hydrocarbons (C_{20}-C_{27}). Components in the cyclone dust are distributed across the entire boiling range analyzed.

Ash Pan Water - The major components in the eluted organics from ash pan water are:

- Chlorinated alkane (4%)
- Dichlorophenol (6%)
- Alkyl benzene (6%)
- Unsaturated hydrocarbons (22%) (BP near 300°C)
- Sulfur (S_8) (15%)

Product Gas Combustion Emissions - The major components in the eluted organics from the product gas combustion emission are:

- Benzaldehyde (6%)
- Ethyl styrene (8%)
- Naphthalene (15%)
- Aromatic compound (6%)
- Unsaturated hydrocarbon (18%) (retention time of 25.17 min; same as in ash pan water)
- Combined phthalates and adipates (11%)

These substances account for 64% of the eluted organics. It cannot be ascertained which species (other than the plasticizers) might not originate with the combustion gas.

ESP Oil Combustion Emissions - The major components found in the eluted organics from ESP Oil combustion emissions are:

- Phthalates and adipates (plasticizers) (58%)
- Naphthalene (6%)
- Methyl indan (4%)
- Unsaturated hydrocarbon (retention time of 25.17 min) (6%); also found in samples from other streams
- Long chain alkanes, C_{21}-C_{27} (13%)

The first component on the ESP oil combustion emission list, identified as trichloropropane, represented 2% of the elution response. The origin of the compound is unknown. It is not a normally encountered solvent impurity, and its presence in the combustion gas is unexpected.

Priority pollutants in the organics from the respective streams tested during the Foster-Wheeler/STOIC gasifier study are listed in Appendix C, Table C-6. Two components common to all streams were naphthalene, associated with gasification and combustion processes, and phthalate (plasticizer), an artifact of sampling and sample handling. The relatively large amount of plasticizer contamination in the product gas organics is probably the result of multiplying a "determined value" by a large dilution factor needed for the GC-MS analyses. In this way, a comparatively small amount of contaminant in the sample would be indicated as a large quantity in the stream.

Stream flow rates given in Appendix A were used to calculate mass flows of the priority pollutants given in Table 11. These results indicate that after correcting for phthalates, the three discharge streams (gasifier ash, cyclone dust, and ash pan water) show no significant difference in the rate at which they discharge organic priority pollutants. Further, these results

TABLE 11. MASS FLOW OF PRIORITY POLLUTANTS IN PRODUCT AND DISCHARGE STREAMS, FOSTER-WHEELER/STOIC

(ug/sec)

Compound	Product Streams		Discharge Streams					
	ESP Oil To Boiler No. 3	Combined Product Gas	Cyclone Dust	Gasifier Ash	Ash Pan Water	Combustion Emissions from Product Gas Boiler	Combustion Emissions from Boiler No. 3	Sum of Emissions
Phenol	6.0E5	3990	ND[a]	ND	0.03	17.3	125	142
2,4-dimethylphenol	ND	2.4E4	ND	ND	ND	ND	ND	ND
Naphthalene	7.8E4	7410	0.35	0.35	0.003	43.9	66.7	111
1-methylnaphthalene	1.3E5	7125	ND	ND	ND	6.54	7.5	14
2-methylnaphthalene	9.2E4	5990	ND	ND	ND	5.60	7.1	12.7
Dimethylnaphthalene	6.2E5	2.2E4	ND	ND	ND	6.54	5.4	12
Phenanthrene	8.8E4	295	ND	ND	ND	1.49	3	4.5
Anthracene	6.0E4	209	ND	ND	ND	ND	ND	ND
Fluorene	8.0E4	27	ND	ND	ND	1.68	2.0	3.68
Pyrene	ND	114	0.008	ND	ND	0.65	1.92	2.58
Benzo(a)anthracene	6.0E4	ND	ND	ND	ND	ND	ND	ND
Bis(2-ethyl hexyl) phthalate	5000	1140	ND	1.4	0.06	23.4	83.4	108
Total	1.8E6	7.2E4	0.054	1.75	0.093	107	302	411
TOTAL (corrected for phthalates)	1.8E6	7.1E4	0.054	0.035	0.033	84	219	303

[a] ND = not detected.

TABLE 12. ORGANIC AND PRIORITY POLLUTANTS FROM THE RILEY GASIFIER

Compound(s)	Product Gas Aerosols		Product Gas Vapors	Gasifier Ash	Cyclone Dust	Ash Pan Water
	ug/g[a]	ug/Nm^3	ug/Nm^3	ug/g	ug/g	ug/L
Acenaphthene					0.8	
Acenaphthylene			24,800			2.0
Benzo(a)pyrene	1,450	5,400			1.5	
Bis(2-ethyl hexyl)phthalate	172	640	5,640	3.47		11.1
Chrysene/benz(a)anthracene	1,270	4,730		0.25	2.2	2.4
Diethyl phthalate	137	510	1,710	0.14	0.7	1.9
Di-n-butyl phthalate			1,200	0.11		1.4
2,4-Dimethylphenol			3,160			
Fluoranthene	426	1,590	2,820	0.12	0.8	1.7
Fluorene			11,100			1.0
Naphthalene			41,900	0.13	1.5	7.4
Phenanthrene/anthracene	389	1,450	15,400	0.06	0.9	2.2
Phenol					11.2	241.
Pyrene	544	2,030	2,900	0.12	0.7	1.7
Non-priority pollutants	10,900	40,800	193,000	0.45	41.5	75.9
Sum Quantified[b]	1.5E4[c]	5.7E4	3.04E6	4.8E0	6.2E1	3.5E2
Organic Loading	8.8E5	3.3E6	5.8E6	2.4E2	5.6E3	1.2E4
Percent Quantified[d]	1.7%	1.7%	5.2%	2.0%	1.1%	2.9%

[a] ug of compound per gram of aerosol collected.
[b] By GC-MS.
[c] 1.5E4 = 1.5 x 10^4.
[d] Percentage of extractable organics of each stream quantified by GC-MS.

indicate that the discharge rate of these priority pollutants is about 2.5 times greater from ESP oil combustion than from product gas combustion. The major difference between the oil combustion and product gas combustion emissions was seen in the phenol concentrations at 30 and 3.7 ug/m^3, respectively.

Organics from the Riley Gasifier

Detailed analyses of organics from the Riley gasifier were limited to the determination of specific organic priority pollutants by GC-MS. The components identified, given in Table 12, represent 1-5% of the total organics as determined by the Level I screening (TCO and GRAV). Many of the components identified were found in the other gasifiers.

Organics from the Wellman-Galusha Gasifier (Fort Snelling)

An objective of the Wellman-Galusha test at Ft. Snelling was to use the organic screening as a prioritization step for a phased approach to an environmental assessment. As a result, the speciation focused on the identification and quantification of selected species in the organics and their respective LC fractions. In this test, components were detected, identified, and quantified by GC-MS (Table 13). Numerous compounds of concern were shown not to be produced at detectable levels. A major portion of identified species of concern were transported on the product gas particulates. These species represented less than 0.2% of the mass of total organics as determined by the Level I screening (TCO + GRAV). Many of the specific compounds determined in the product gas were present in other gasifiers (e.g., alkyl benzenes and polycyclics). However, the identified nitro compounds had not been reported previously from other gasification systems. More generally identified are nitrogen heterocyclic compounds and arylamines. The distributions of compounds across the respective LC fractions indicate that the procedure functioned as desired, having the aromatics in fraction 2 and the polar nitrogen compounds in the later fractions. Organics from the test burner flue gas showed only benzoanthracenes, reported as benzo(a)anthracene, at a concentration of 4.5E 2 ug/m^3.

TABLE 13. PRIORITY POLLUTANTS IN LC FRACTIONS OF ORGANICS FROM THE PRODUCT GAS OF THE WELLMAN-GALUSHA (FORT SNELLING) GASIFIER (ug/m^3)

	Organics on Particulates (Aerosols)					Sum of Particulates Organics	Organic Vapors			Sum of Organics Vapors	Sum of Condensable Organics	Product Gas Total
	LC-2	LC-3	LC-4	LC-5	LC-6		LC-2	LC-3	LC-4			
Benzene												>1.3E4
Thiophene												1.9E3
Toluene												2.6E2
C_2-alkyl benzenes												1.4E2
Benzo(a)anthracene	2.8E1	1.7E3				1.7E3	8.1E0	1.4E2		1.4E2	1.8E3	1.8E3
Benzo(b)fluoranthene	1.0E1	3.7E2				3.8E2		1.0E1		1.0E1	3.9E2	3.9E2
Polychlorinated biphenyls[a]	≤7.6E0					≤7.6E0	≤7.2E0				≤7.2E0	≤1.5E1
Biphenyl		1.2E2				1.2E2		5E3		5E3	5.1E3	5.1E3
7,12-Dimethylbenzo(a)anthracene		1.6E2				1.6E2					1.6E2	1.6E2
Benzo(c)phenanthrene		9.7E2				9.7E2		6.5E1		6.5E1	1.0E3	1.0E3
Benzo(a)pyrene		1.9E2				1.9E2					1.9E2	1.9E2
Methyl chloranthene		4.7E0				4.7E0					4.7E0	4.7E0
Dibenzo(a,h)anthracene		6.1E0				6.1E0					6.1E0	6.1E0
Dinitrotoluene			2.2E3			2.2E3					2.2E3	2.2E3
Dinitrocresol				8.4E2		8.4E2			9.8E2	9.8E2	1.8E3	1.8E3
Dihydroacridene				2.3E1	9.1E1	1.1E2					1.1E2	1.1E2

[a] Source - Tables D79 and D85 indicate present but below quantification limit (10).

Organics from the Wellman-Galusha Gasifier (Glen Gery)

The detailed analyses for the Glen Gery gasifier consisted primarily of GC-MS analyses. The results listed in Table 14 are based on a limited search for selected compounds presumed to be of concern.

The organics from the particulate collected from the product gas (column 2, Table 14) are based on micrograms of organics per gram of particulate. To express this mass in terms of product gas volume, each value must be multiplied by the gas stream particulate loading of approximately 0.0015 ug/m^3, which reduces the listed values by three orders of magnitude. Therefore, in terms of product gas total organic loading, the quantity of organics borne by the particulates is relatively small. The summed organics in the product gas (441 ug/m^3), corrected for sulfur and plasticizer, equal approximately 220 ug/m^3. This is significantly lower than the levels of similar components in the product gas from other fixed-bed processes operating on lignite or bituminous coal. These identified organics represent only a small portion of the total organic loading (7000 ug/m^3) being transported in the gas stream.

Organics from the Lurgi-Type (Kosovo) Plant

Detailed analyses in the Kosovo study were performed by GC-MS for selected polynuclear aromatics (PNA), by GC-FID for phenols, and by element specific detector GC for nitrogen- and sulfur-bearing organics.

PNAs--

The PNA data are shown in Table 15. The varying minimum levels (<n) shown for the PNAs are related directly to the sample preparation and the extent of concentration of each extract since the mass spectrometer maximum sensitivity was constant at about 0.1 ppm in the measured solution. Higher sensitivities were attained in some samples (e.g., 0.085 ug/m^3 or 8pptr in the naphtha storage tank vent condensate) by evaporative concentrations. These results indicate that the benzo(a)pyrene (BaP) concentration of the naphtha is

TABLE 14. CONCENTRATIONS OF SELECTED POLLUTANTS IN VARIOUS STREAMS AND SEPARATE SAMPLES FROM WELLMAN-GALUSHA (GLEN GERY) GASIFIER

	Product Gas Vapors (ug/m^3)	Product Gas[a] Aerosols (ug/g)	Cyclone Dust (ug/g)	Particulates Inlet Air (ug/g)		Gasifier Ash-Dry (ug/g)	Gasifier Ash-Wet (ug/g)	Ash Water (ug/L)	Combustion Gas (ug/m^3)
				Day 1	Day 2				
Ancenaphthalene	6								
Anthracene phenanthrene	25	20	0.1		0.50				0.4
Fluoranthene	6	7	0.1		0.25				0.4
Fluorene	6				0.25				
Naphthalene	75		0.4	0.7	0.8				1.2
Phenol	52	ND(0.07)[b]	ND(0.01)	ND(0.03)	ND(0.03)	ND(0.0001)	ND(0.001)	ND(0.7)	6.9
Methyl Phenol ≥2 Isomers	27								
Dimethylphenols	11								
Bis(2-ethylhexyl)phthalate	8	200	2.0	1.0	0.25	0.58	0.03	33	47
Pyrene	15	20							0.6
Sulfur[c]	210	4000	160	ND(0.03)	ND(0.03)	77	30	ND(0.07)	ND(0.02)
Chrysene/Benzanthracene		7							
Phenols		ND(0.7)	ND(0.01)						
D-N-Butylphthalate		20	0.2	0.7	0.25	0.08	0.34	7	
Diethyl Phthalate		20	0.2	2.1	1.0	2.1 1.0	0.05	0.15	
Chloronaphthalene				0.3					
Butylbenzylphthalate					0.50				
Benzo(a)pyrene									0.8
Sum of Species by GC-MS	441	4274	163	4.8	4.5	77.7	30.5	40	15
Total Organic Loading	6990	25,100	785	242		116	96	46,500	1900
% Volatile Organics	9.7	18.7	5.4	49		11.2	34.4	86.0	50
% Non-volatile Organics	90.3	81.3	94.6	51		88.8	65.6	14.0	50
% of Total Organics Speciated	6.3	17	21	2		67	32	<0.1	0.8

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[a] The particulate loading in the product gas is approximately 1500 ug/m^3.

[b] ND means not detected but if present would be below indicated level (detection limit).

[c] From Appendix of Reference 5.

TABLE 15. PNAs IN LURGI-TYPE (KOSOVO) STREAMS

	7.12 dBaA[a]	BaA[b]	BbF[c]	BaP[d]	dBahA[e]	3-meC[f]	252[g]
Gaseous Streams (ug/m^3)							
LP Coal Lock Vent		163	670	670	52		
Ammonia Stripper Vent		85	12	20	<2.1[h]		
Naphtha Storage Tank Vent		<0.06	0.11	0.085	0.06		
Start-Up Vent		--[i]	--	139	<2.1		
Tar Tank Vent		--	--	252	<10		
Phenolic Water Tank Vent		--	--	<50	<50		
Medium Oil Tank Vent		--	--	<6.5	<6.5		
H_2S-Rich Waste Gas		--					
CO_2-Rich Waste Gas		--	--	<0.7	<0.7		
Organic By-Products (ug/g)							
Heavy Tar	1300	500	320	240	14	NF[j]	1000
Light Tar	1100	490	310	210	23	26	950[k]
Medium Oil	62	160	120	68	7	NF	280[k]
Naphtha	NF	NF	NF	NF	NF	NF	NF
Aqueous Streams (ug/mL)							
Phenolic Water[l]	0.23	0.92	0.68	0.19	0.02	<0.004	1.3
Phenosolvan Waste Water	NF	NF	NF	NF	NF	NF	0.19

[a] 7,12 dBaA = 7,12-Dimethylbenz(a)anthracene
[b] BaA = Benz(a)anthracene
[c] BbF = Benzo(b)fluoroanthene
[d] BaP = Benzo(a)pyrene
[e] dBahA = Dibenz(a,h)anthracene
[f] 3-meC = 3-Methylchloranthrene
[g] 252 = 252 group as BaP
[h] All (<) values are calculated from a minimum detectable concentration of 0.1 ppm in solution.
[i] -- = Not detected at 1 ug/g.
[j] NF = None found.
[k] BaP = 24% of group of compounds at molecular weight = 252 in both by-products.
[l] Phenosolvan feed: also referred to in this report as gas liquor.

perhaps less than 0.1 ppm but greater than 8 pptr. The major source of PNA emission from the Kosovo plant was the coal lock vent gas that discharged 670 ug/m^3 of BaP; at a representative flow rate of 21 m^3/hour from each gasifier vent, the mass flow rate of BaP would be 3.9 ug/gasifier-second.

Phenols--

The phenol data (Appendix C Table 7) were obtained from the acid extractable fraction of each of the various streams. This fraction should contain primarily phenolic compounds; consequently all GC peak areas were quantitated as phenol (i.e., using the response factor for phenol). Several observations can be made from these data:

- The identified portion of the eluted mass ranges from 23% in tar to 69% in the organics extracted from phenolic water.
- The unidentified peaks listed in the table (Appendix C Table C-7) most likely represent alkyl phenols because there are a total of six possible dimethyl isomers that boil between 211°C and 237°C and there are many other higher alkyl phenols that would elute after the 2,4-dimethyl isomer but within the retention range of the unidentified peaks.
- If the total acid fraction eluting from the GC is due to phenolic components, then 17% of the tar and 23% of the medium oil is phenolic.
- The speciated phenols in the phenolic water sum to about 2700 mg/L. This is in agreement with the colorimetric determination of 2120 mg/L (total phenolics).

Sulfur-Bearing Species--

Analyses were conducted for mercaptans in 13 gas streams (Appendix C Table C-8) and in the head space over the major by-products and organic wastes (Appendix C Table C-9). Although higher boiling sulfur-bearing species were observed on some chromatograms, the compounds were not quantified because a universal calibration factor could not be applied reliably with the flame photometric detector used for the analyses, and no standards were available for the unidentified higher boiling sulfur species. Therefore, the results do not include all of the volatile sulfur species. Tentative identifications for thiophenes were made by peak enrichment and by correlating retention times with published boiling points (Appendix C Table C-10). The compounds listed do not include all of the eluting peak areas of the chromatograms but rather the major components indicated by clearly resolved GC peaks. Quantification was based on an assumed linear detector response to sulfur by electrical conductivity. These sulfur species, present in virtually all process and discharge streams that contain some level of condensable organics, are distributed between the various streams according to solubility and vapor pressure.

Nitrogen-Bearing Species--

The major nitrogen-bearing species contained in the by-product medium oil and phenolic water were tentatively identified as pyridines, alkyl pyridines, quinoline, and alkyl quinolines. The quantified species (Appendix C Table C-11) provide a partial (about 15%) accounting of the one percent nitrogen content of the medium oil and an indication of the nitrogen-bearing compounds present.

Organics from the Texaco Gasifier (Ruhrkohle/Ruhrchemie in Oberhausen-Holten)

Aqueous Samples--

Detailed analyses by GC and/or GC-MS for 67 priority pollutants in the settler underflow (during two test periods) showed virtually no organic compounds discharged from the gasifier except for a trace of phenol. Phenol, not detected by the water quality analyses (EPA 420.1 - detection limit 0.18 mg/L), was detected in the sample from Test 2 by GC-MS and quantified at 0.0026 mg/L by GC-FID.

Solid Phase Samples--

Organic compounds detected in solid phase samples are tabulated (ug/g) below:

Component	Sludge		Settler Fines	
	Test 1	Test 2	Test 1	Test 2
Bis-2-ethyl hexyl phthalate	170	ND	5	570
Di-n-butyl phthalate	ND	ND	4	ND
n-alkanes (C_{10}-C_{30})	ND	1.0	ND	ND
Benzoic acid	ND	ND	11.0	ND

It is likely that the phthalates occurred from sampling and laboratory handling after the sample was withdrawn from the system. The benzoic acid concentration shown above is only about 2 times the limit of detection. It is evident from these results that organics from the aqueous and solid streams of the Texaco gasifier are low compared to fixed-bed processes.

Organics from the Koppers-Totzek Gasifier (Modderfontein)

The thrust of this test was to make an environmental assessment of the aqueous streams; consequently only limited information is available from the process (Appendix C Tables C-12 and C-13). The major effort to characterize organics was done by a screening test that provided estimates of concentration by chemical classes based on low resolution mass spectrometry and priority pollutant detection by GC-MS. These appended results show few compounds identified at substantial levels. PNAs which were positively identified and quantified by HPLC are tabulated below:

	Rectisol Condensate	
Compound	Sample 1 (ug/L) 11/12/79	Sample 2 (ug/L) 11/19/79
Fluoranthene	24	17
Pyrene	32	25
1,2-Benzofluorene	15	15
1,2-Benzoanthracene	23	16
Benzo(k)fluoranthene	2	2

In addition to these compounds, five unidentified PNAs having molecular weights of 230, 242, and 252 were present. Using a combination of GC-MS and high performance liquid chromatography it was established that benzo(a)pyrene (MW = 252) was not one of these unidentified components.

Organics from the Bi-Gas Gasifier (Homer City, Penn.)

Volatile organic species (listed in Appendix C Table 14) were identified by GC-MS in several gas streams of the Bi-Gas process. However the level of organics in the product gas is low compared to the various tar-producing processes. It is apparent that the major portion of these volatile aromatics are removed from the product gas by the Selexol process and transported with the acid gas. A novel heterocyclic compound, 1,2,3,4,5-pentathiopane, an eight-membered ring with five sulfurs and 2 methylene units, was tentatively identified at trace levels among these organics.

Organics from the KRW-Fluidized Bed Gasifier (Madison, PA)

The test of this process development unit (PDU) differed from most other tests included in this report. The major difference between this test methodology and that used for the other gasifiers was the omission of the determination and characterization of organic loading by the procedure for a Level I Environmental Assessment (18). By the Level I procedure volatile organics (Total Chromatographable Organics), non-volatile organics (GRAV), and light hydrocarbons are defined by the analytical procedures and are divided into three groups: light hydrocarbons (C_2-C_6), volatile organics (boiling points equivalent to C_6-C_{12}) and non-volatile organics (boiling point greater than C_{13}).

The methodology used in this study reported volatile hydrocarbons between C_6 and C_{10} and semivolatile organics as species having a molecular weight greater than 128; benzene was reported separately. Since boiling point and chromatographic retention time may be correlated with each other but not with molecular weight, the definitions used in the KRW report are substantially different from those provided by the Level I procedure. In order to reconcile these differences all organic species determined by GC-MS were summed to obtain a value for total organics. It must be recognized that these chromatographable organics do not include non-chromatographable organics that would be determined in the (GRAV) fraction of the Level I procedure. Nevertheless, the data can provide a valuable insight into the relationship between the organics produced by this process and those produced by fixed bed processes.

In this section the composition and loading of the organics as determined by GC-MS in the product gas will be discussed; comparisons with fixed bed processes will be made.

Organics in Product and Recycled Gas Streams--

Volatile organics in the crude product gas from the KRW-PDU include ethane and benzene at the ppmv level plus other higher boiling organics at the ppbv level. The results, summarized in Table 16, show concentrations and mass flows of the predominant condensable organic species as benzene (300-400 ppmv) which is present at a level several orders of magnitude greater than the combined higher boiling constituents. Other light aromatics, e.g., toluene (0.5 ppmv) and xylene (<0.1 ppmv), are present at such low levels that they do not affect the overall result. The only light hydrocarbon detected was ethane which also was present at the ppmv level. It is apparent that the mass of total organics produced by the KRW gasification process is dominated by the mass of benzene and ethane.

Detailed analytical data, as obtained by GC-MS on samples of gas produced from three different fuels - bituminous coal, subbituminous coal and lignite - are provided in Appendix C, Tables C-15, C-16, and C-17, respectively. A summary of these detailed results are shown in Appendix C Table C-18. Several observations can be made about these data and also of the mass flow data shown in Table 16:

TABLE 16. SUMMARY OF ORGANICS DATA FROM KRW'S PROCESS DEVELOPMENT GASIFICATION UNIT

	Units	Type of Coal		
		Bituminous	Subbituminous	Lignitic
Coal Feed Rate	Kg/hr	500	650	780
Raw Product Gas Flow Rate	m^3/hr	930	1160	1520
Summation of Organic Species	ug/m^3	520	240	220
Organic Mass Flow Rate	g/sec	1.3E-4	7.8E-5	9.4E-5
Organics Produced per Coal	g/ton	1.0E0	4.3E-1	4.3E-1
Benzene Concentration	ug/m^3	4.5E5	1.6E6	1.1E6
Benzene Mass Flow Rate	g/sec	1.2E-1	5.2E-1	4.6E-1
Benzene Produced per Coal	g/ton	8.3E2	2.9E3	2.1E3
Ethane Concentration	ug/m^3	NA[a]	2.1E5-2.1E6	3.3E5
Ethane Mass Flow Rate	g/sec	NA	7.0E-2-7.0E-1	1.4E-1
Ethane Produced per Coal	g/ton	NA	3.8E2-3.8E3	6.4E2

[a] NA = not analyzed.

- Concentration levels of organics (220 - 520 ug/m^3) based on the summation of species are significantly lower than those obtained from similar analyses of product gas from other fixed bed gasifiers (Chapman 7.4E4, Foster-Wheeler/STOIC 5.1E5 ug/m^3).

- These concentration levels, obtained by summing species, are well below the total organic loadings in product gas from fixed bed gasifiers which averaged 8.6 g/m^3 as determined by the Level 1 methodology.

- The concentration of organics in product gas from the KRW gasifier was similar for all three fuels tested.

- The production rate of organics is also similar for all three fuels tested.

- Within each coal test, the concentrations of individual species are not consistent across the several gas streams tested and the differences do not seem to correlate with cooling or blending.

- Variation observed in the number of species detected in the respective streams is most likely due to concentrations at or near the detection limits of the techniques:

	Number of Species Detected		
	Bituminous Coal	Subbituminous Coal	Lignite
Raw Product Gas	19	13	16
PG Cooler Exit	21	8	13
RG Cooler Exit	27	9	22
Test Cooler Exit	19	16	12

- Many of the species detected in KRW product gas-organics were also found in product gases-organics from other processes. However, a few sulfur compounds such as pentathiocyclohexane had not been reported previously. It is not known whether these unique compounds were not present in organics from other processes or if they had not been identified.

In the KRW report, volatile organics were defined as components having molecular weights less than 128. However, components having molecular weights up to 148 were quantified and included in the tabulation of organics (22). Several compounds were reported both with the volatile organics and with the semi-volatile organics. Samples for the two determinations were collected differently: volatile organics were collected on Tenax while semi-volatiles were collected on XAD-2 resin. A point of concern is the observed difference in the concentration levels of components common to both groups because the concentrations in the volatile groups are at the ppmv level while the same compound in the semi-volatile group is at the ppbv level. The following tabulation illustrates the concern:

Naphthalene Concentration (ppb)

	Reported as Semi-Volatile Organics		Reported as Volatile Organics		
Type of Coal	(ppb)	N[a]	(ppb)	N[a]	Range (ppb)
Bituminous	22	1	430 ± 822[b]	5	16-1900
Subbituminous	30	1	5000	1	-------
Lignitic	18	1	64 ± 84[b]	6	ND(<1.6)-180

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[a] = Number of determinations.
[b] = Standard Deviation.

Consequently, the large differences between samples and/or sampling methods present a concern as to the true value of any indicated concentration and the large difference within a set of samples (b above) suggests strongly that the methodology used was not capable of reliable measurement at the concentrations encountered. As a result, any datum based on a single measurement should be viewed only as an indicator of concentration level and not as a determination of concentration. In those cases where large differences are found between successive samples of a given stream it is not possible to determine from the reported data whether those differences are the result of variations within the process, heterogeneous samples, or non-reproducible measurement.

Organics in KRW Process Water--

Data for TOC, COD, oil and grease and phenol in several aqueous streams of the KRW Process are reported in Appendix C Table C-19. These values were obtained by the methods for water quality parameters using replicate samples (generally 3 but sometimes 2) for three different types of coal. The values entered for the KRW Process in Table 6 were obtained by averaging and rounding-off these data from bituminous and subbituminous coals. The data from the lignite tests show significant scatter. It cannot be stated with confidence that the differences between the means for the bituminous and subbituminous coal test are very significant. For example, the TOC mean value of 90 ± 2.1 for the quench water from bituminous coal would appear to be higher than the mean value of 77 ± 3.1 from subbituminous coal. However, the intervals overlap at the 95% confidence level. Although these data do not allow quantitative comparisons between streams or fuels with that high level of certainty, they do show conclusively that the levels of organics are significantly lower than those found in quench water from fixed bed gasifiers.

Extractable organic species as determined by GC-MS are shown in Appendix C Tables C-20, C-21, and C-22. Highest concentrations were found in the water from the separator pit where the sum of the organics totaled 20 mg/L (Table C-21). Phenol was found in most of the streams tested at concentrations between 100 and 600 mg/L with subbituminous coal as the fuel. Phenol levels were generally lower (10-100 ug/L) using the other fuels. Volatile organics measured included benzene at the 0.1-20 ppm level, pyridine at the 50 ppb level and naphthalene at the 1-100 ppb level (Appendix C Table C-23). Of the four aqueous streams tested, benzene concentrations were the highest in separator pit water at 1 ppm for bituminous and subbituminous coals and 18 ppm for lignite.

Organic Species in Solids From The KRW Gasification Process--

Organic species determined in solids from the KRW Gasification process are shown in Appendix C Table C-24. Highest concentrations found were for naphthalene (300-600 ppm for all fuels). Benzo(a)pyrene (1.9 ppm) was detected on particulates from the product gas produced with bituminous coal. Gasifier ash showed sub ppm levels of organics. Those found were primarily long straight chain hydrocarbons.

SECTION 6

ORGANIC PROFILES

A major deficiency of the detailed quantitative analysis data from complex coal gasification streams is that it is incomplete (i.e., only a portion of the total organics can be identified without extremely costly and prolonged analyses). Comparisons between similar streams of different processes or different streams of the same process may not be possible when only a small portion of components are included in the quantitative data. A useful and cost effective technique that provides a profile for comparison is "fingerprinting." One of the simplest fingerprints is a gas chromatogram using an FID as in Figure 24 which shows the distributions of hydrocarbons in the major by-products from the Lurgi-type plant at Kosovo. The commonality and distributions of components are clearly evident. Also useful are gas chromatograms using element-specific detectors to provide profiles of the sulfur- or nitrogen-bearing components.

The fingerprint data do not lend themselves to computer storage and retrieval as easily as do quantitative data, but they provide an informative description of the complex mixtures produced by fixed-bed gasifiers. This information is not readily evident in the detailed quantitative data from GC-MS. These profiles show that the long lists of compounds detected by GC-MS do not necessarily convey the great molecular complexity of the organics associated with coal gasification processes. Included in this array of hydrocarbons are heteroatomic compounds, compounds containing either oxygen, nitrogen, or sulfur in addition to carbon and hydrogen and also di- or multi-hetero hydrocarbons, compounds containing combinations of nitrogen, sulfur, and oxygen in addition to carbon and hydrogen.

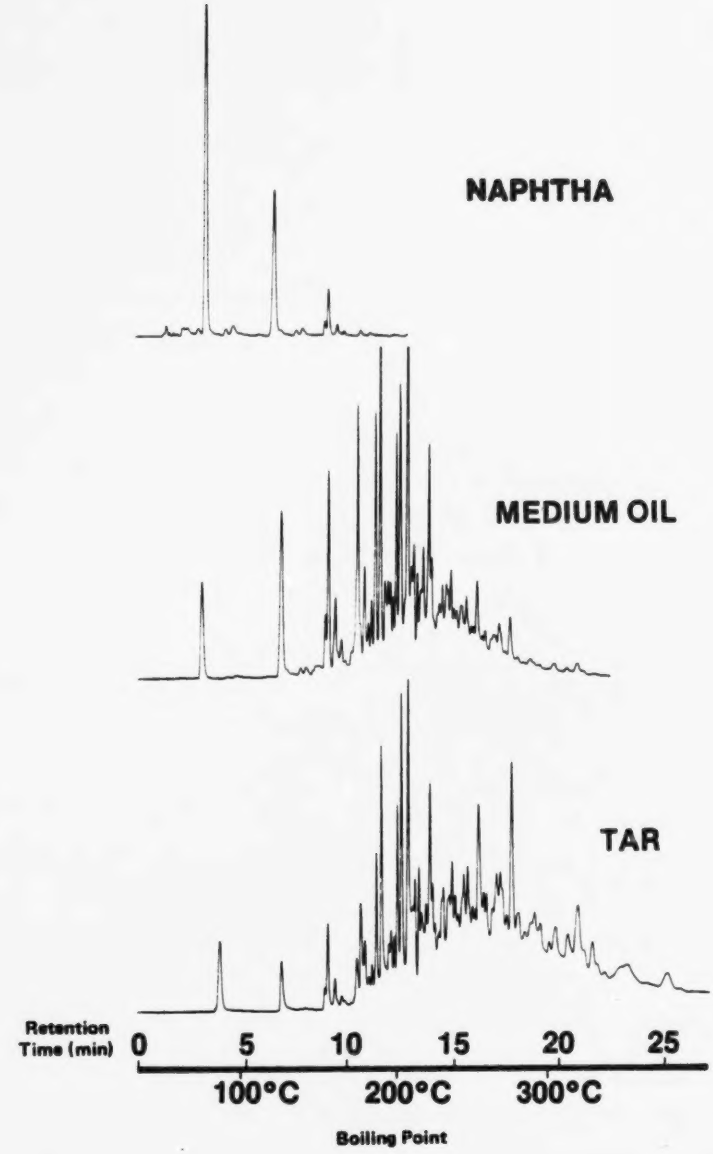


Figure 24. GC-FID chromatographic profiles of the major by-products from the Lurgi-type (Kosovo) gasifier.

Such profiles were obtained for several gas stream condensates from the Kosovo plant. For example, Figure 25 shows the nitrogen specific chromatogram of the condensable organics from four gaseous discharge streams. It is evident that the discharge from the LP coal lock (representative of crude product gas) and the other discharges contain similar distributions of nitrogen-bearing organics. These compounds have been identified tentatively as pyridine, alkyl pyridines, quinoline, and alkyl quinolines. Since the response of this detector is generally linear, each chromatogram provides a normalized basis for the chromatographable organic nitrogen. The retention time provides an indication of the boiling range of the species.

Figure 26 shows chromatograms of nitrogen-bearing species in three fractions of medium oil. The sample oil contains organic bases such as the pyridines and quinolines found in the gas stream condensates. However, the separation shows that the mixture is much more complex containing acidic (base extractable), neutral, and basic nitrogenous compounds. Many neutral and acid extractable compounds could fall within the boiling point range projected on the chromatograms in Figure 26. In this respect, tentative assignments of component types such as pyridines, quinolines, alkyl arylamines, pyrazines, and pyridizines/pyrimidines are plausible.

Figure 27 shows a chromatogram of nitrogen species from a fraction that precipitated out of the medium oil during the acid extraction. This fraction, reconstituted by basifying, is believed to be a mixture of pyrroles. Pyrroles were not reported in the GC or GC-MS analyses of Kosovo organics yet the classical splint test for pyrroles (20) was positive, indicating they are present in medium oil. The peak in the chromatogram labeled carbazole (dibenzopyrrole) was identified tentatively by enrichment (co-elution) with the known compound.

These chromatographic profiles illustrated the complexity of nitrogen-bearing substances which may be produced by gasification. If the same acid, base, and neutral fractions of medium oil are scanned for sulfur-bearing species, it is evident that the mixture is even more complex. Figure 28 shows that the acid extractables, in addition to pyridines, contain sulfur-bearing

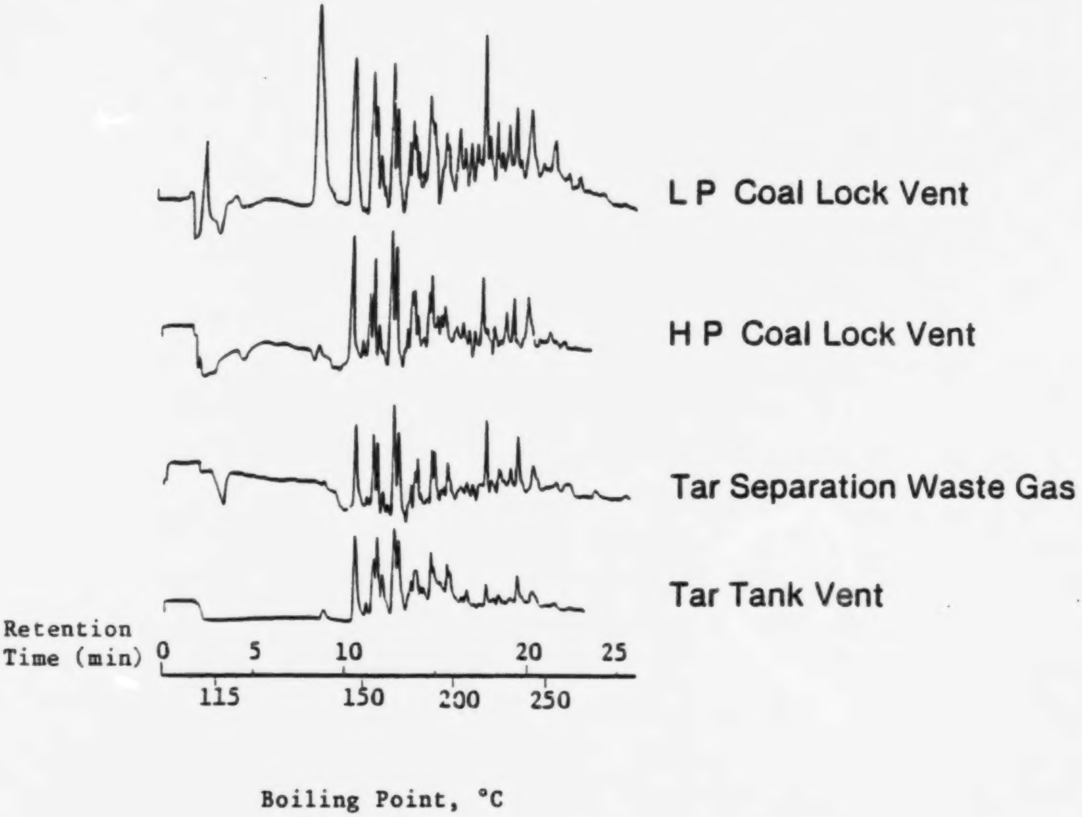
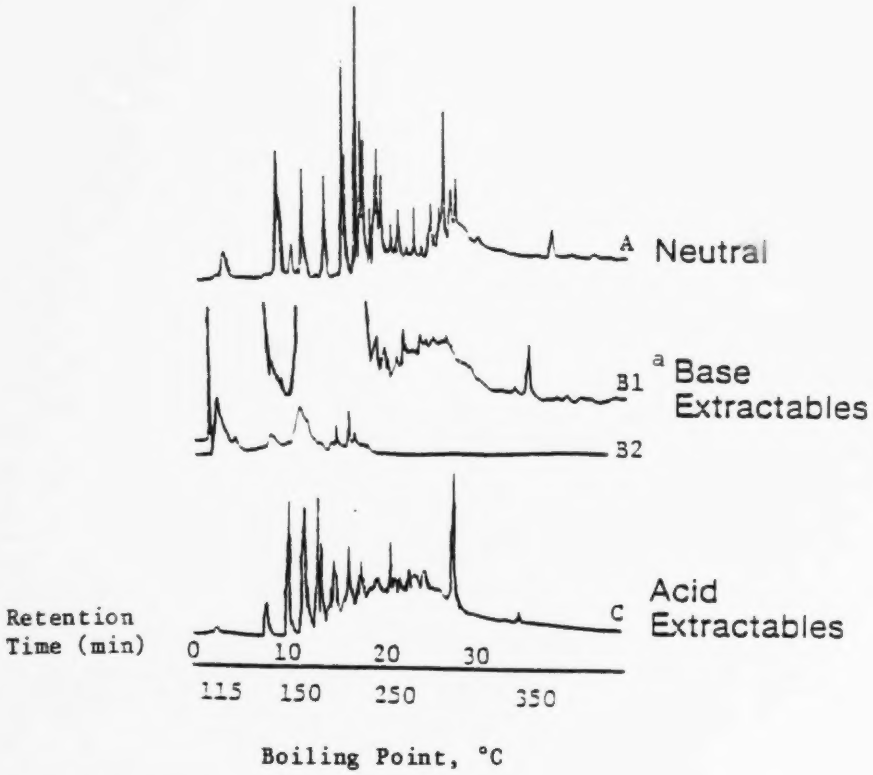
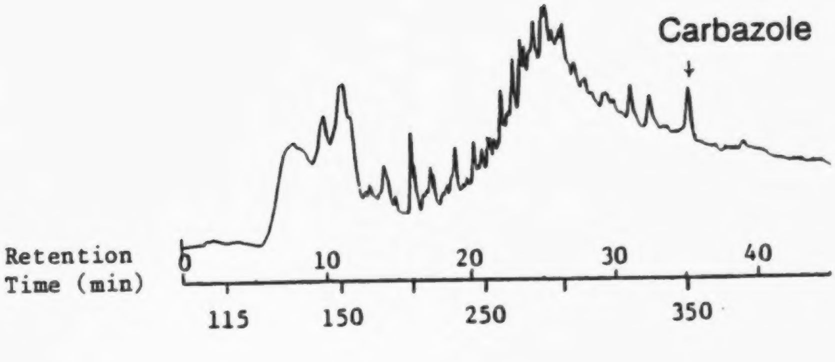


Figure 25. Chromatograms of nitrogen species in condensates from four Kosovo streams.



[a] Sample size of B1 >> B2

Figure 26. Chromatograms of nitrogen species in Kosovo medium oil.



Boiling Point, °C

Figure 27. Chromatogram of nitrogen species in the material that precipitated from medium oil during acid extraction.

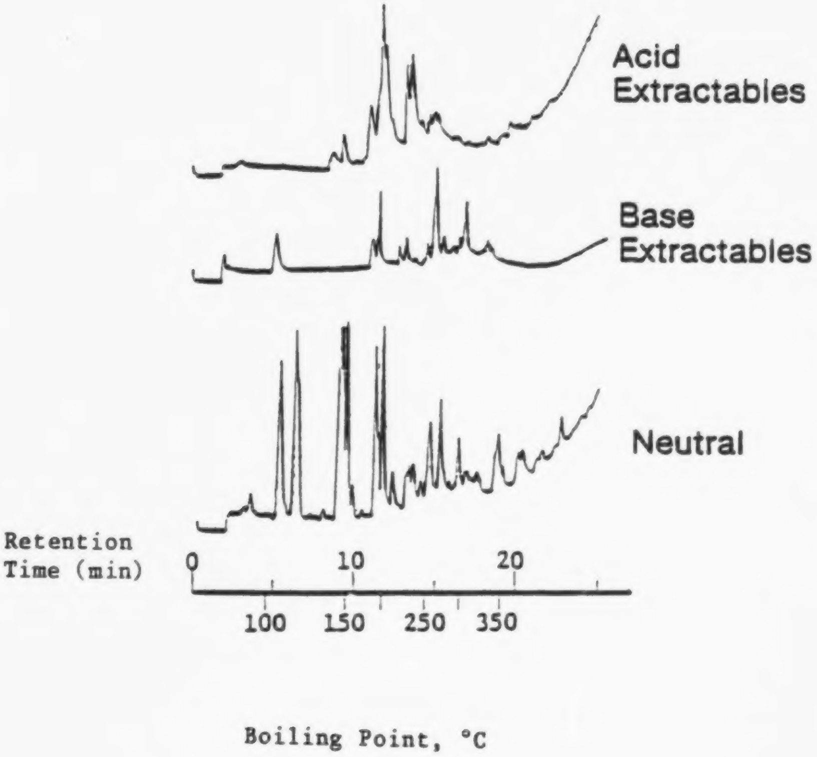
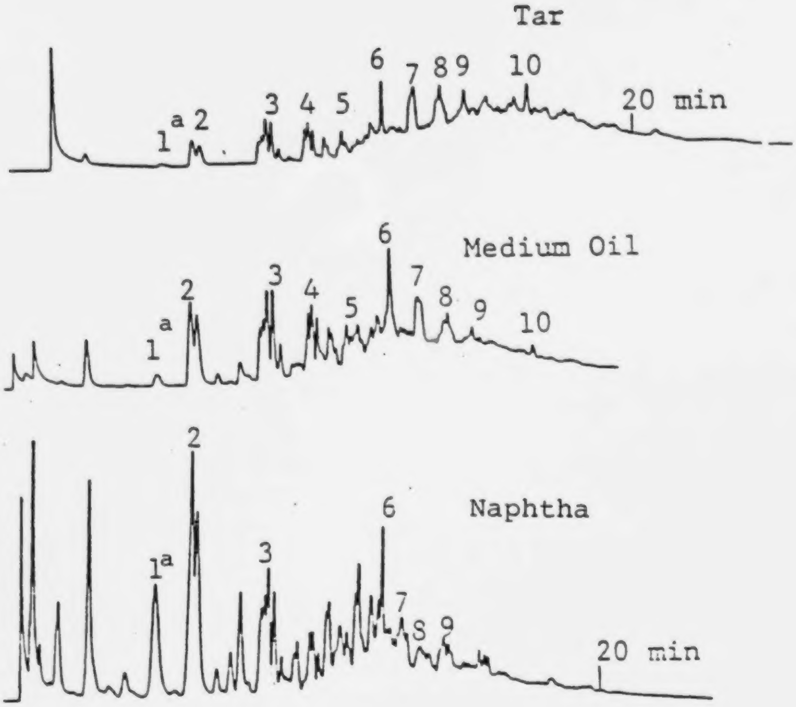


Figure 28. Chromatograms of sulfur species in Kosovo medium oil.

substances in the boiling range between 150 to 350°C. These substances contain both nitrogen and sulfur. The neutral fraction contains alkylthiophenes while the base extractable fractions undoubtedly contain thiophenols or possibly hydrothiophenes. The thiophenes are the dominant sulfur-bearing species of the unfractionated organic by-products as is evident in Figure 29 where chromatographic profiles of the sulfur-bearing species in medium oil, tar, and naphtha are compared. The numerals identify peaks and peak clusters that are similarly retained and are therefore of similar composition. It is apparent that all these by-products contain many of the same species but that distributions and boiling point range differ.

The chromatograms in Figure 30 show distributions of nitrogen-bearing species in gas liquor from the two tar-producing sources which were most extensively characterized, the Lurgi-type (Kosovo) and the Chapman gasifiers. The numbers above each peak indicate the actual retention times of the component. Used as fingerprints, these chromatograms show that the two gas liquors contain many of the same nitrogenous components. The major difference is that the Chapman liquor contains a greater amount of quinoline (2 rings) relative to pyridines (1 ring) than the Lurgi-type gas liquor.



[a] Peaks identified with the same numeral have closely similar retention times and are likely to have similar composition.

Figure 29. Sulfur species in Kosovo organic by-products.

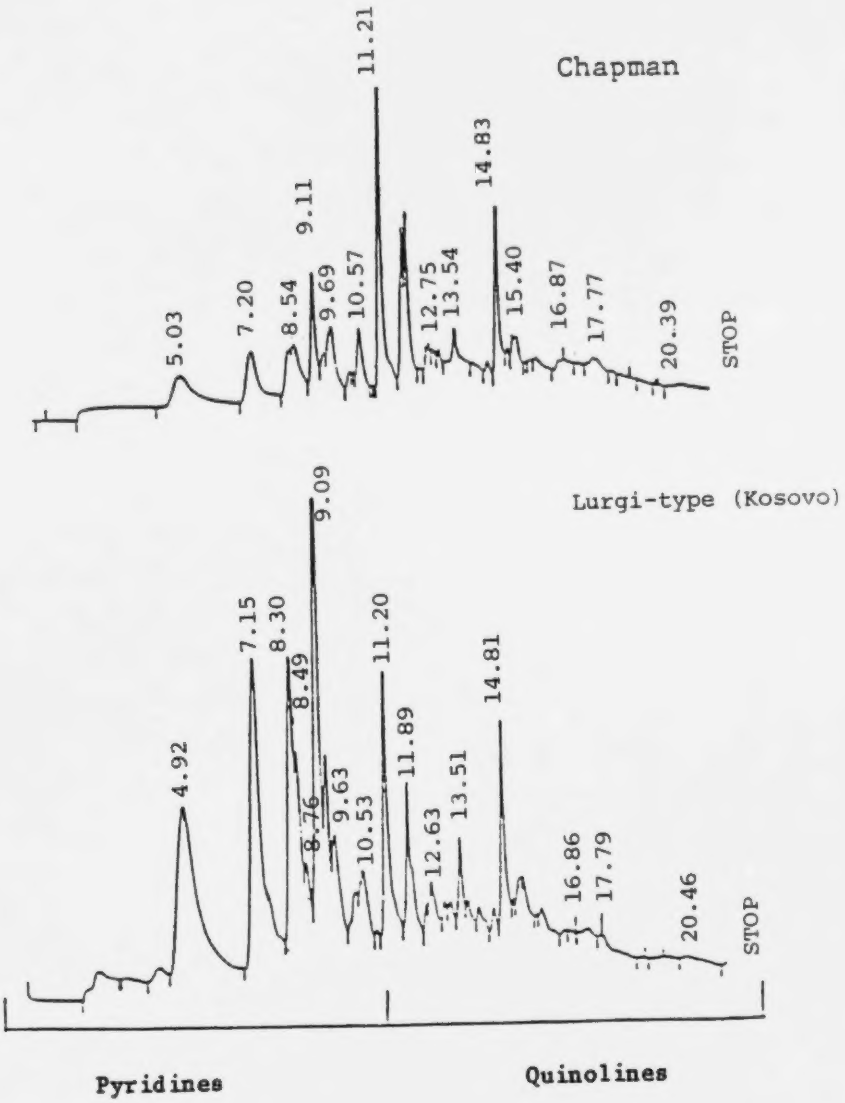


Figure 30. Chromatograms of nitrogen-bearing species in gas liquor from two different plants. Reprinted with permission of the copyright owner (21).

SECTION 7

INTERNAL QUALITY CONTROL

The data compiled in this summary report originated from a series of Source Test and Evaluation projects conducted over a period of several years. During this time span the measurement techniques and quality control requirements were modified and evolved such that no single consistent set characterizes all of the data. However, the quality control procedures described below are generally applicable to the data types included in this report.

The internal quality control (QC) system for these data provided a set of routine internal procedures for assuring that the data output met prescribed criteria for data quality. Inherent and implied in this control function was a parallel function of measuring and defining the quality of the data output. A well-designed internal QC program must be capable of controlling and measuring the quality of the data, in terms of precision and accuracy. Precision reflects the influence of the inherent variability in any measurement system. Accuracy reflects the degree to which the measured value represents the actual or "true" value for a given parameter, and includes elements of both bias and precision. Accuracy of measurement data is related to the precision and bias of the component parts of the measurement system.

Generally, the internal QC procedures may be divided into two overlapping categories. One category includes those procedures which were used to control data quality within the prescribed limits of acceptability. These acceptability limits are usually related to data precision, accuracy, and completeness. The other category includes those procedures designed to provide a quantitative assessment of data quality, again in terms of precision, accuracy, and completeness. Some internal QC procedures, by their nature, fall into both categories.

PROCEDURES USED FOR CONTROL AND ASSESSMENT OF DATA QUALITY

Those procedures which served both control and assessment functions first come to mind when quality control is mentioned. Examples include:

- replicate and repeat analyses (split samples),
- blanks analyses,
- replicate samples,
- control samples,
- drift checks,
- spiked samples, and
- QA audits.

Procedures of this type were performed at a specified frequency, with a requirement that specific acceptance criteria be met prior to proceeding with sample analyses. Failure to meet prescribed acceptance criteria indicated the need for corrective action. By selecting appropriate acceptance criteria for QC results, the quality of the measurement data was effectively controlled within predetermined limits. Since precision and accuracy are most frequently the quality aspects which were being controlled, acceptance criteria for these types of procedures were defined in terms related to precision and accuracy. An essential part of the control function is the requirement that all acceptance criteria be met prior to proceeding with actual sample analyses. Table X-1 is an example of a summary of internal QC requirements for the testing programs which includes designated frequencies and specific acceptance criteria for each procedure.

In addition to controlling data quality within prescribed limits, the QC data provided the basis for assessing the performance of the measurement system. This assessment, usually involving statistical treatment of the QC data, was used to define various aspects of measurement data quality, including precision and accuracy. One major advantage of the types of procedures listed above is the ongoing nature of this assessment which represents a powerful feedback mechanism in a corrective action scheme. In order to maximize this potential, the data should be plotted and/or tabulated on a routine basis. Control charts are often used for this purpose, with some variation of the Shewhart chart being the most popular type of control chart.

ADDITIONAL DATA QUALITY ASSESSMENT PROCEDURES

In addition to the QC checks described above, which provided both ongoing assessment and control of the measurement system, other QC procedures were used in what is, practically speaking, strictly an assessment function. Any control benefits of these types of QC procedures are realized only over the long term, as through modification or refinement of procedures and techniques. Examples of these evaluative procedures include:

- collaborative tests,
- methods validation studies,
- interlaboratory (round-robin) analyses,
- analysis of variance studies, and
- method comparisons.

These types of QC procedures were not included in the day-to-day QC system, but rather were used for specific applications. They are especially suited to projects which involve methods development or which require modification of standard methods for a particular novel measurement application or situation.

ADDITIONAL DATA QUALITY CONTROL PROCEDURES

The QC procedures described above are oriented to quantitative data QC in the sense that there is an obvious and direct link between each procedure and some measureable aspect of data quality. Another type of QC procedures served a control function which was more qualitative rather than quantitative.

Strict adherence to prescribed measurement procedures falls into this category, and is often the single most important QC procedure in terms of overall impact on measurement data quality. Other examples of this type of QC procedure include:

- training of personnel,
- preventive maintenance,
- documentation,
- calibration/standardization procedures,
- data review and calculation checks,
- use of formatted data forms which serve as checklists,
- careful consideration in experimental design,
- data reduction procedures, and
- statistical data evaluation.

Since much of the early organic characterization included in this report was of a qualitative and semi-quantitative nature, the QC procedures used fall into this latter category. In some cases the techniques described in the first category were used, but only for a portion of the methodology. For example, replicate analyses were employed in the laboratory to a single grab sample so that only a portion of the variance could be assessed. In some cases, such as in the Kosovo study, geopolitical factors prevented a strict adherence to a comprehensive QC program. However, the confidence level of the data was enhanced by combining the results of several independent tests which, while not as worthy as a rigorously applied test matrix, was vastly superior to a single measurement of a single sample.

Since the initial objective of the test for a Level I Environmental Assessment as employed in this work was to determine whether a more definitive analysis was needed, the values for organic loading that are reported and compared were not intended to be used as a final statement of composition or quantity. Because there is a tendency among technologists to try to get as much out of a datum as possible, there is an urgent need to recognize that virtually all values contained in this report were obtained for use as indicator values and that only a few were obtained and reported as accurately measured concentrations. It must also be recognized that the concentrations and mass flows reported here were obtained at fixed points in time and therefore may not represent the full range of normal operation, nor the operating norm. Nevertheless, the data reported provide a basis for evaluating and comparing coal gasification processes in terms of the organics in their respective process and discharge streams.

The quality control procedures that evolved during the course of this series of tests are summarized in Tables 17, 18, and 19.

TABLE 17. SUMMARY OF INTERNAL QUALITY CONTROL PROCEDURES FOR LIQUID AND SOLID PHASE SAMPLES

Parameter	Analytical Method	Quality Control Check	Frequency	Acceptance Criteria	Action or Corrective Action
Extractable Organics*	Gravimetric	Methylene chloride	Prior to sample analyses	None	Used to indicate level of analytical contamination
		Duplicate analyses	10% (minimum 1)	None	Report results

TABLE 18. SUMMARY OF INTERNAL QUALITY CONTROL PROCEDURES FOR AQUEOUS SAMPLES

Parameter	Analytical Method	Quality Control Check	Frequency	Acceptance Criteria	Action or Corrective Action
Total Organic Carbon (TOC)	EPA/415.1	Method blank (DI water)	Prior to sample analyses	None	Used to indicate level of analytical contamination
		Control sample	1) Immediately following calibration 2) 10% (minimum 2) thereafter	Percent recovery between 85-115%	1) Repeat control sample analysis 2) Repeat calibration and sample analyses back to valid control sample analysis
		Duplicate analyses	10% (minimum 1)	Relative percent difference (RPD) ≤20% for replicate determinations	Repeat duplicate analysis
		Impinger blank	Minimum 1	None	Will be used to determine amount of contamination
Biochemical Oxygen Demand (BOD)	EPA/405.1				
Chemical Oxygen Demand (COD)	EPA/410.1	Method blank (DI water)	Prior to sample analyses	None	Used to indicate level of analytical contamination
		Control sample	10% (minimum 2)	Measure value within ±15% relative error (RE) of true value	1) Repeat control sample analyses 2) Repeat sample analyses back to last valid control sample analysis
		Duplicate analyses	10% (minimum 1)	Relative percent difference (RPD) <20% for replicate determination	Repeat duplicate analysis
Total Phenolics	EPA/420.1	Method blank	Prior to sample analyses	None	Used to determine analytical contamination
		Control sample	10% (minimum 1)	Measure value ±15% relative error (RE) of true value	1) Repeat control sample analysis 2) Repeat sample analyses back to last valid control sample analysis
		Duplicate analyses	10% (minimum 1)	Relative percent difference (RPD) ≤20% for replicate determinations	Repeat duplicate analysis
		Sample spikes	10% (mimimum 1)	Spike recovery between 80-120%	Repeat spike analysis
		Impinger blank	Minimum 1	None	Will be used to determine amount of contamination

TABLE 19. SUMMARY OF INTERNAL QUALITY CONTROL PROCEDURES FOR GAS PHASE SAMPLES

Parameter	Analytical Method	Quality Control Check	Frequency	Acceptance Criteria	Action or Corrective Action
Organic Gases C_2 - C_6	GC/FID	Linearity check (multi-point calibration) species of interest	Initially	Correlation coefficient >0.98 for each parameter of interest	Repeat calibration
		Single point RF check	Daily, prior to sample analysis using mid-level standard	RF for each parameter of interest within ±20% of the calibration RF	1) Repeat single point analysis 2) Repeat calibration
		Control sample	Daily (minimum 2), prior to sample analysis and at conclusion	Agreement with control sample theoretical concentration within ±20% for each parameter of interest	1) Repeat control sample analysis 2) Repeat calibration and reanalyze samples back to last valid control sample analysis
		Duplicate analysis	10%; minimum of 2 samples per batch	Relative percent difference (RPD) ≤30% for 90% of the qualified peaks	Repeat sample analysis back to last valid control check
		Method blank	Daily prior to sample analyses (nitrogen)	Less than five times detection limits	1) Clean system 2) Repeat blank analysis 3) Repeat single point RF check
		Field blanks	Minimum 1	None	Will be used to determine sources of contamination
Sulfur Gases (H_2S, SO_2, COS, CS_2, CH_3SH, C_2H_5SH, $(CH_3)_2$, and Thiophene)	GC/FPD	Generation of (multi-point calibration curves	Initially	None	
		Single point RF check	Daily, prior to sample analyses using mid-level standard	RF for each parameter of interest within ±20% of the calibration RF	1) Repeat single point analysis 2) Repeat calibration
		Control sample	Daily (minimum 2), prior to sample analysis and at conclusion	Agreement with control sample theoretical concentration within ±20% for each parameter of interest	1) Repeat control sample analysis 2) Repeat calibration and reanalyze samples back to last valid control sample analysis
		Method blank	Daily, prior to sample analyses	Less than five times detection limit	1) Clean system 2) Reapt blank analysis 3) Repeat single point RF check
		Field blanks	Minimum 1	None	Will be used to determine sources of contamination

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APPENDIX A

GASIFIER FLOW RATE DATA

TABLE A-1. CHAPMAN GASIFIER STREAM FLOW RATE DATA

Stream	Flow rate, g/s-gasifier[a]
Inputs:	
Coal	152
Air	385
Steam (water vapor)	80
Outputs:	
Cooled product gas	495
Gasifier ash (dry basis)	9.3
Cyclone dust	0.8
By-product tar	15

[a] Average for the two gasifiers.

Source: Ref. 2.

TABLE A-2. WELLMAN-GALUSHA (FORT SNELLING) GASIFIER STREAM FLOW RATE DATA

Stream	Flow rate, g/s-gasifier Sampling Period One	 Sampling Period Two
Inputs:		
Coal	320 ± 28	250 ± 21
Air	500 ± 55	444 ± 49
Steam (water vapor)	67 ± 8.4	66 ± 8.3
Outputs:		
Dry product gas	720 ± 63	570 ± 49
Product gas moisture	130 ± 16	120 ± 15
Tar	12 ± 1.4	9.8 ± 1.1
Gasifier ash	27 ± 2.8	21 ± 2.1
Cyclone dust	3.8 ± 1.3	--[a]
Gasifier ash sluice water	7	7
Cyclone dust quench water	<7	---

[a] -- means not available.

Source: Ref. 10.

TABLE A-3. WELLMAN-GALUSHA (GLEN-GERY) STREAM FLOW RATE DATA

Stream	Flow rate, g/s-gasifier
Inputs:	
Coal	219
Air	992
Steam (water vapor)	194
Outputs:	
Product gas	1,333
Gasifier ash	20.6
Cyclone dust	0.2
Coal hopper gas	2.2
Pokehole gas	1.7

Source: Ref. 5.

TABLE A-4. RILEY GASIFIER STREAM FLOW RATE DATA

Stream	Flow rate, g/s-gasifier
Inputs:	
Coal (including moisture)	1,000 ± 109
Air	1,200 ± 240
Steam	350 ± 88
Service water	2,200 ± 440
Outputs:	
Product gas (dry basis)	2,300 ± 230
Moisture in gas	620 ± 61
Gasifier ash	75 ± 30
Cyclone dust	4 ± 1
Tars and oils	21 ± 4
Ash pan water	2,200 ± 440

Source: Ref. 9.

TABLE A-5. FOSTER-WHEELER/STOIC GASIFIER STREAM FLOW RATE DATA

Stream	Flow rate, g/s-gasifier
Inputs:	
Coal (including moisture)	300 ± 30
Air	620 ± 120
Steam (water vapor)	70 ± 7
Ash pan makeup water	7 ± 4
Lock hopper purge steam	16 ± 4
Pokehole purge steam	6 ± 2
Outputs:	
Combined product gas (dry basis)	930 ± 190
Moisture in product gas	75 ± 15
Gasifier ash	35 ± 4
Moisture in gasifier ash	9 ± 0.9
Cyclone dust	0.2 ± 0.1
ESP oil	4 ± 1

Source: Ref. 11.

TABLE A-6. LURGI-TYPE GASIFIER STREAM FLOW RATE DATA

Stream	Flow rate, g/s-gasifier
COAL PREPARATION	
Run-of-mine coal	6,667
Dryer offgas (dry basis)	22
Dryer condensate	--[a]
Dried coal	4,444
GASIFICATION/GAS QUENCH	
Dried coal	4,444
Oxygen	778
Steam	3,611
High pressure coal lock vent (dry basis)	65
Low pressure coal lock vent (dry basis)	5.6
Ash lock cyclone vent (dry basis)	12.4
Wet ash	750
Ash quench wastewater	720
Crude gas (dry basis)	4,675
RECTISOL AGR	
Crude gas (dry basis)	4,675
Clean product gas (dry basis)	1,275
H_2S-rich offgas (dry basis)	1,758
CO_2-rich offgas (dry basis)	1,725
Cyanic water	172
Naphtha	36
GAS LIQUOR SEPARATION	
Cyanic water	172
Heavy tar	28
Waste gas (dry basis)	12.4
Medium oil	69
Light tar	111
Phenolic water	3,611
PHENOSOLVAN/STRIPPING	
Phenolic water	3,611
Crude phenol	25
NH_3 stripper vent gas	96.5

[a] -- means not available.

Source: Ref. 7.

TABLE A-7. KRW PDU GASIFIER STREAM FLOW DATA

Stream	Flow Rate, g/s-gasifier		
	Test 1 Wyoming Subbituminous	Test 2 Pittsburgh No. 8	Test 3 North Dakota Lignite
Inputs			
Coal	219.2	141.0	271.6
Steam	56.8	73.4	67.2
Oxygen	112.8	145.3	135.6
CO_2 to gasifier	50.8	65.7	49.2
H_2O injection	0.0	150.3	0.0
Coal lockhopper gas (CO_2)	4.0	2.6	5.0
Ash lockhopper gas (CO_2)	1.7	1.7	1.7
Makeup water	479.4	207.9	161.3
Outputs			
Scrubbed and cooled product gas	364.0	321.9	453.8
Gasifier ash	11.6	16.0	15.6
Wastewater	506.1	408.1	202.4
Sludge	51.8	13.8	37.7
Coal lockhopper vent	3.5	2.3	4.2
Ash lockhopper vent	1.7	1.7	1.7

Source: Ref. 22.

TABLE A-8. KOPPERS-TOTZEK GASIFIER STREAM FLOW RATE DATA

Stream	Flow Rate, g/s-gasifier
Inputs:	
Pulverized coal	1,750
Oxygen	1,640
Steam	175
Outputs:	
Raw gas (dry)	3,110
Slag	80
Discharge water	2,275
Fly ash (dry)	210

Source: Ref. 13.

TABLE A-9. TEXACO GASIFIER STREAM FLOW RATE DATA

	Flow rate, g/s-gasifier	
Stream	Period One[a]	Period Two[b]
Inputs:		
Coal (dry basis)	1,690	1,634
Oxygen	1,564	1,561
Fresh water[c]	1,319	347
Demineralized water	1,424	1,278
Outputs:		
Scrubbed synthesis gas	3,221	3,206
Slag	570	501
Flash gas	7.5	8.3
Settler underflow-blowdown	2,141	1,029

[a] No recycle of clarifier underflow.
[b] Minimization of fresh water makeup by recycle of clarifier underflow.
[c] Includes water in coal feed, additive mixture, and flocculant mixture.

Source: Ref. 12.

APPENDIX B

DETAILS OF SELECTED SAMPLING AND ANALYTICAL TECHNIQUES

This appendix contains more detailed explanations of the techniques used to analyze Chapman, Foster-Wheeler/STOIC, and Riley gasifier samples for organics.

ANALYSIS AND QUANTIFICATION OF THE CHAPMAN ORGANICS BY GC-MS

Extracts and extract fractions of Chapman organics were analyzed using a Hewlett-Packard Model 5980 GC-MS system equipped with a Model 5930 data processing system.

The analytical conditions used for all extracts and fractions except the free phenol fraction were:

- Carrier: He, 25 mL/min
- Oven Program: 60°C to 300°C at 8°C/min with an initial hold of 2 min and a final hold of 8 min
- Analytical Column: 1.8m x 2mm ID glass column packed with 1% SP-2100 on 100-120 mesh Supelcoport
- MS Span: 40-320 m/e
- MS Span Time: 3 sec

The phenols were analyzed under the same conditions except that the analytical column was packed with 60-80 mesh Tenax GC.

Concentration approximations were based on peak height measurements from the total ion plot. Peak heights were compared to the peak height of d_{10}-anthracene spiked into the final extract concentrates at 20 ng/uL as an internal standard. Concentrations of individual compounds in the extracts were calculated using the following equation:

$$C = \frac{a \times 20}{b \times c}$$

where: C = concentration of a compound in the extract in ng/uL

a = peak height of the compound of interest in the total ion plot

b = response factor of the compound of interest relative to d_{10}-anthracene

c = peak height of d_{10}-anthracene at 20 ng/uL

If the response factor (RF) for the compound of interest was known, that RF was used. If the RF was not known, an RF of 1 was assumed except for phenols. An RF of 0.4 was used for all phenols as a conservative approximation of their actual RFs. A list of compounds along with their known RFs relative to d_{10}-anthracene is given in Table B-1.

GC-MS ANALYSIS OF ORGANICS FROM THE FOSTER-WHEELER/STOIC GASIFIER

Composited extracts were analyzed using gas chromatography-mass spectrometry (GC-MS). The samples were analyzed for the base-neutral and acid extractable EPA Priority Pollutants given in Table B-2 using a computer assisted search. This technique searches for specific compounds based on the appearance of three characteristic fragment ions within a known relative retention time window. Quantitation was done by response factor comparison to a known amount of d_{10}-anthracene.

TABLE B-1. RESPONSE FACTORS RELATIVE TO d_{10}-ANTHRACENE USED IN GC-MS DATA CALCULATIONS

Compound	Response Factors
Naphthalene and alkyl derivatives	0.637
Acenaphthylene and alkyl derivatives	0.783
Acenaphthene and alkyl derivatives	0.483
Fluoranthene and alkyl derivatives	0.837
Benz(a)anthracene	1.26
Benzoperylene	1.04
Phenols	0.4
All others	1.0

TABLE B-2. BASE/NEUTRAL AND ACID EXTRACTABLE PRIORITY POLLUTANTS ANALYZED BY GC-MS

Base/Neutral Extractable

Compound	m/e
1. 1,3-Dichlorobenzene	146
2. 1,4-Dichlorobenzene	146
3. Hexachloroethane	117
4. 1,2-Dichlorobenzene	146
5. Bis(2-Chloroethyl) ether	93
6. Bis(2-Chloroisopropyl) ether	121
7. Nitrobenzene	77
8. N-Nitrosodimethylamine	74
9. N-Nitrosodi-n-propylamine	130
10. Hexachlorobutadiene	225
11. Isophorone	82
12. 1,2,4-Trichlorobenzene	180
13. Bis(2-Chloroethoxy) methane	93
14. Naphthalene	128
15. Hexachlorocyclopentadiene	237
16. 2-Chloronaphthalene	162
17. Acenaphthylene	152
18. Acenaphthene	154
19. Dimethyl phthalate	163
20. 2,6-Dinitrotoluene	63
21. 4-Chlorophenyl phenyl ether	204
22. Fluorene	166
23. 2,4-Dinitrotoluene	63
24. Diethyl phthalate	149
25. N-Nitrosodiphenylamine	169
26. 1,2-Diphenyl hydrazine	77
27. Hexachlorobenzene	284
28. 4-Bromophenyl phenyl ether	248
29. Phenanthrene	178
30. Anthracene	178
31. Di-n-butyl phthalate	149
32. Fluoranthene	202

Base/Neutral Extractable (cont'd.)

Compound	m/e
33. Pyrene	202
34. Benzidine	184
35. Butyl benzyl phthalate	149
36. Bis(2-Ethylhexyl) phthalate	149
37. TCDD	322
38. Chrysene	228
39. Benz(a)anthracene	228
40. 3,3-Dichlorobenzidine	252
41. Di-n-octyl phthalate	149
42. Benzo(b)fluoranthene	252
43. Benzo(k)fluoranthene	252
44. Benzo(a)pyrene	252
45. Indeno(1,2,3-c,d)pyrene	276
46. Benzo(a,h)anthracene	278
47. Benzo(g,h,i)perylene	276

Acid Extractable

Compound	m/e
1. 2-Chlorophenol	128
2. 2-Nitrophenol	139
3. Phenol	94
4. 2,4-Dimethylphenol	12
5. 2,4-Dichlorophenol	162
6. 2,4,6-Trichlorophenol	196
7. p-Chloro-m-cresol	142
8. 2,4-Dinitrophenol	184
9. 4,6-Dinitro-o-cresol	198
10. Pentachlorophenol	266
11. 4-Nitrophenol	139
12. 2,2-Difluorobiphenyl	190

Samples were analyzed by GC-MS using the following parameters:

Instrument:	Hewlett-Packard 5985 GC-MS system
Column:	30 meter SE-54 fused silica capillary
Carrier:	Hydrogen at 35 cm/sec
Injector Temperature:	250°C
Oven Program:	25°C for 3 min; 16°C/min to 60°C and 6°C/min to 300°C
Ionizing Voltage:	70 eV

GC-MS ANALYSIS OF THE RILEY GASIFIER ORGANICS

GC-MS analyses were carried out on organic extracts from the product gas, gasifier ash, cyclone dust, ash pan water, and service water of the Riley gasifier to provide qualitative and quantitative data for specific organic compounds. The analyses used a computer assisted GC-MS system for the EPA Priority Pollutants. Priority pollutant analyses were performed as a rapid and cost-effective means to identify and quantify specific compounds of potential concern, such as a number of the polynuclear aromatics.

In addition to priority pollutant analysis, the major non-priority pollutant peaks in each sample were quantified assuming a response factor of 1.0 relative to d_{10}-anthracene. This provided a more complete characterization of the organic compounds in the samples since many compounds of potential health and ecological concern are not priority pollutants.

Finally, the total unidentified chromatographable mass in each extract was quantified by relating the concentration of identified compounds to the total organic loading. If a worst-case assumption was made for the unidentified mass in each sample, these data could be used to indicate the need for further detailed sample characterization.

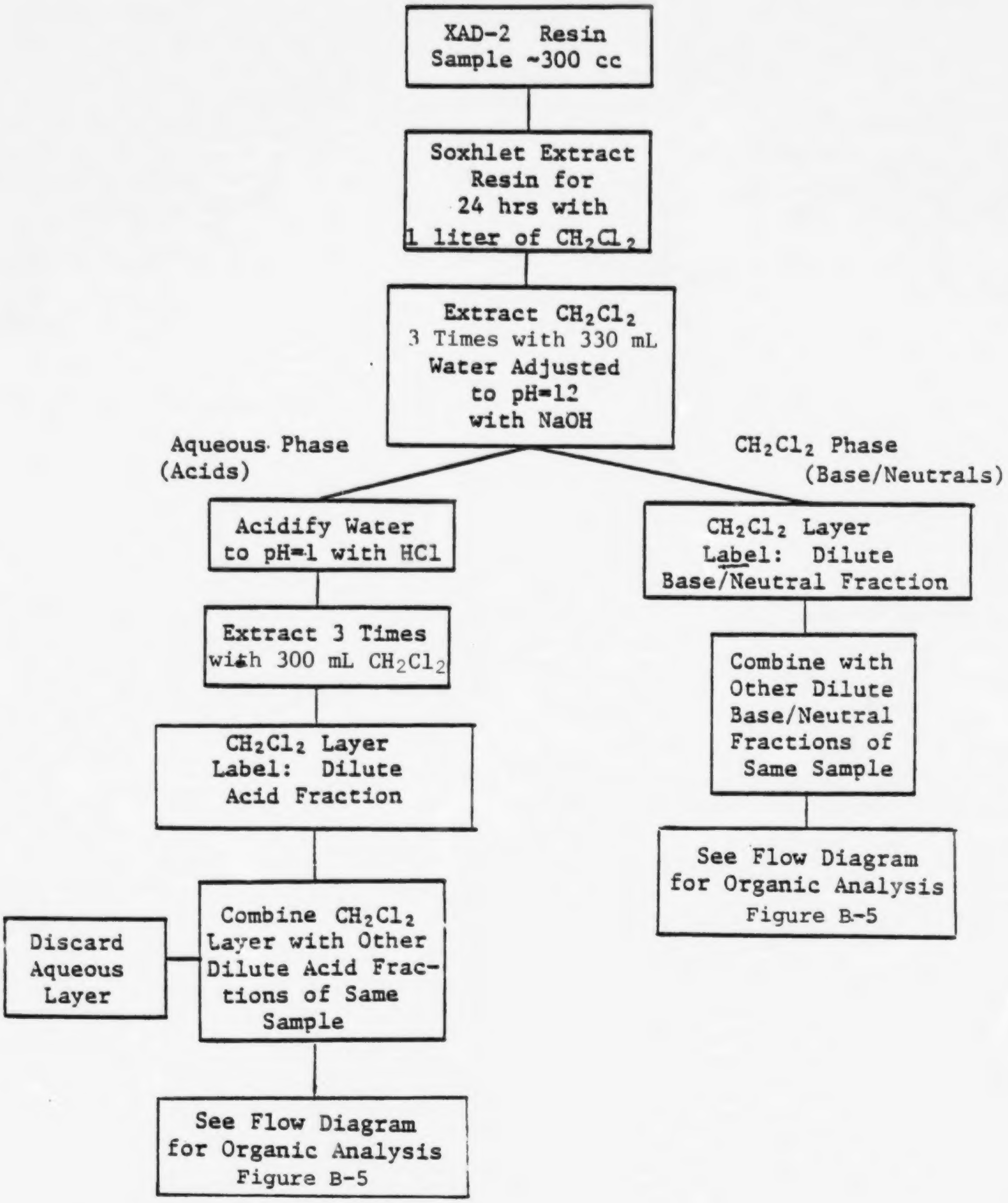

XAD-2 Resin
Sample ~300 cc
Soxhlet Extract Resin for 24 hrs with 1 liter of CH_2Cl_2
Extract CH_2Cl_2 3 Times with 330 mL Water Adjusted to pH=12 with NaOH
Aqueous Phase (Acids)
CH_2Cl_2 Phase (Base/Neutrals)
Acidify Water to pH=1 with HCl
Extract 3 Times with 300 mL CH_2Cl_2
CH_2Cl_2 Layer Label: Dilute Acid Fraction
Discard Aqueous Layer
Combine CH_2Cl_2 Layer with Other Dilute Acid Fractions of Same Sample
See Flow Diagram for Organic Analysis Figure B-5
CH_2Cl_2 Layer Label: Dilute Base/Neutral Fraction
Combine with Other Dilute Base/Neutral Fractions of Same Sample
See Flow Diagram for Organic Analysis Figure B-5

Figure B-1. XAD-2 resin extraction flow scheme.

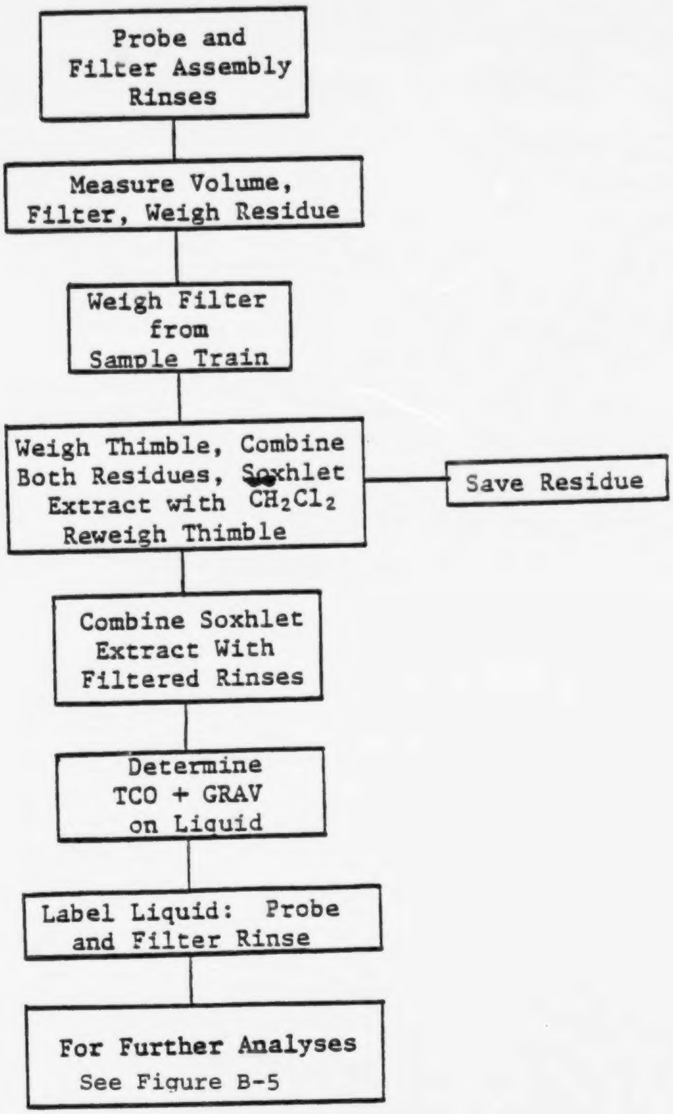

Probe and Filter Assembly Rinses
Measure Volume, Filter, Weigh Residue
Weigh Filter from Sample Train
Weigh Thimble, Combine Both Residues, Soxhlet Extract with CH2Cl2 Reweigh Thimble
Save Residue
Combine Soxhlet Extract With Filtered Rinses
Determine TCO + GRAV on Liquid
Label Liquid: Probe and Filter Rinse
For Further Analyses See Figure B-5

Figure B-2. Flow scheme for the preparation of sample train rinses.

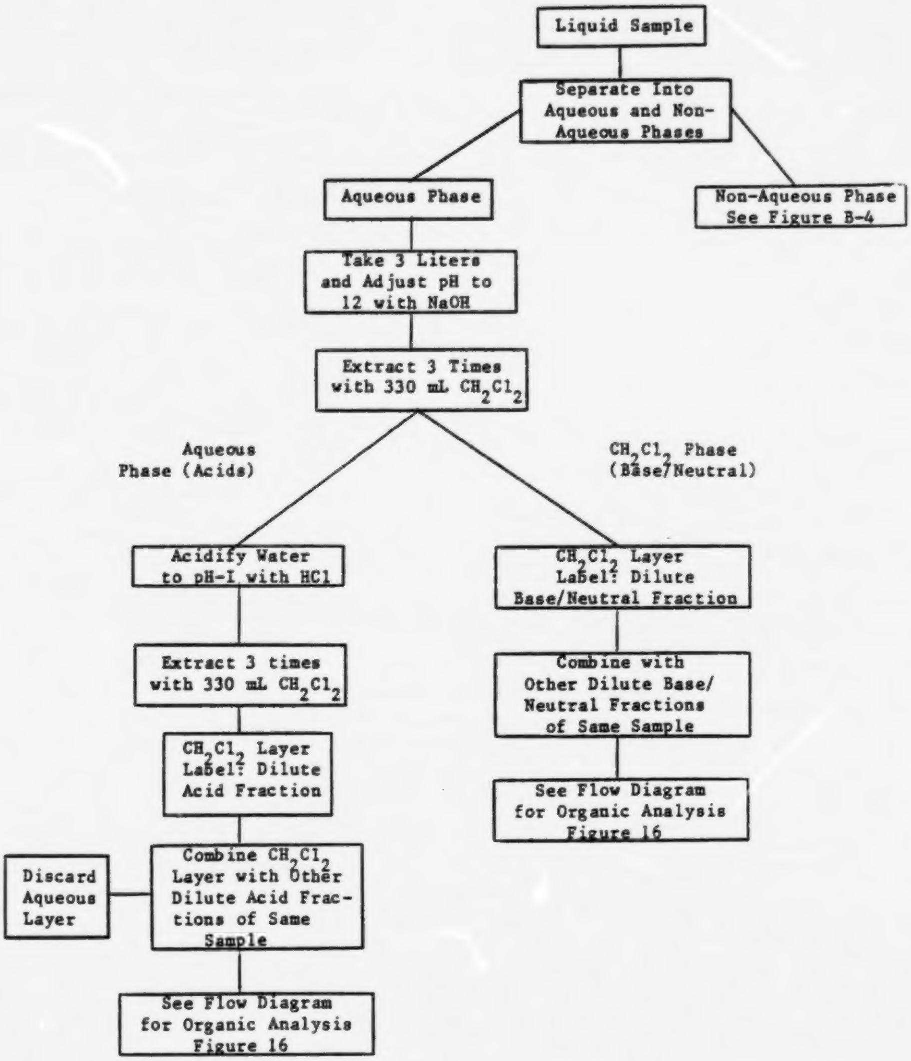

Liquid Sample
Separate Into Aqueous and Non-Aqueous Phases
Aqueous Phase
Non-Aqueous Phase See Figure B-4
Take 3 Liters and Adjust pH to 12 with NaOH
Extract 3 Times with 330 mL CH_2Cl_2
Aqueous Phase (Acids)
CH_2Cl_2 Phase (Base/Neutral)
Acidify Water to pH-I with HCl
CH_2Cl_2 Layer Label: Dilute Base/Neutral Fraction
Extract 3 times with 330 mL CH_2Cl_2
Combine with Other Dilute Base/Neutral Fractions of Same Sample
CH_2Cl_2 Layer Label: Dilute Acid Fraction
See Flow Diagram for Organic Analysis Figure 16
Discard Aqueous Layer
Combine CH_2Cl_2 Layer with Other Dilute Acid Fractions of Same Sample
See Flow Diagram for Organic Analysis Figure 16

Figure B-3. Flow scheme for the extraction of aqueous samples.

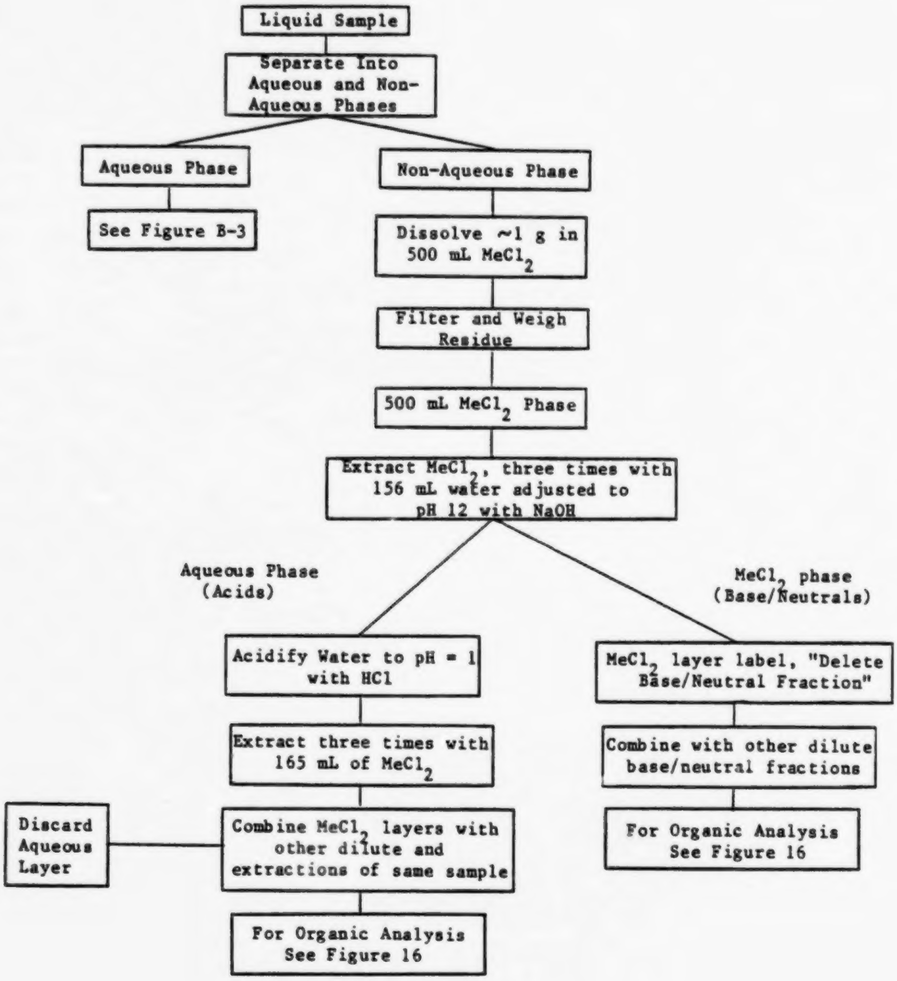
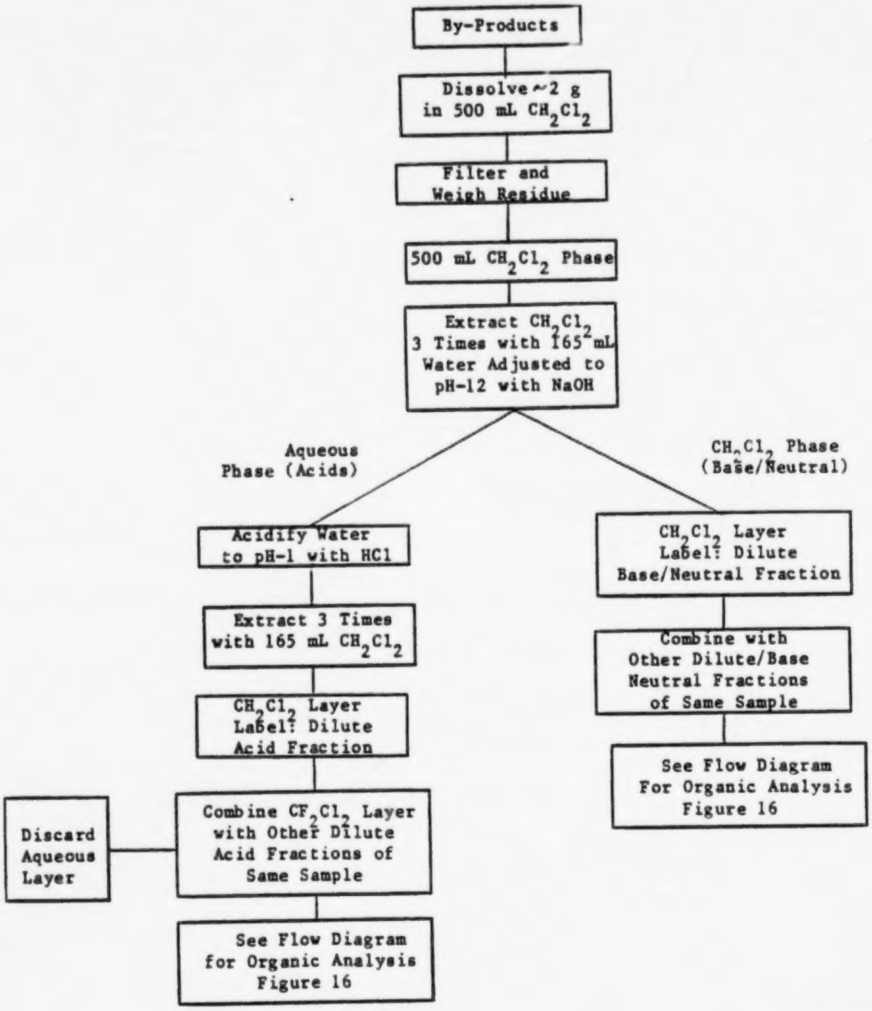

Liquid Sample
Separate Into Aqueous and Non-Aqueous Phases
Aqueous Phase
Non-Aqueous Phase
See Figure B-3
Dissolve ~1 g in 500 mL MeCl$_2$
Filter and Weigh Residue
500 mL MeCl$_2$ Phase
Extract MeCl$_2$, three times with 156 mL water adjusted to pH 12 with NaOH
Aqueous Phase (Acids)
MeCl$_2$ phase (Base/Neutrals)
Acidify Water to pH = 1 with HCl
MeCl$_2$ layer label, "Delete Base/Neutral Fraction"
Extract three times with 165 mL of MeCl$_2$
Combine with other dilute base/neutral fractions
Discard Aqueous Layer
Combine MeCl$_2$ layers with other dilute and extractions of same sample
For Organic Analysis See Figure 16
For Organic Analysis See Figure 16

Figure B-4. Flow scheme for the extraction of non-aqueous phase samples.



By-Products
Dissolve ~2 g in 500 mL CH2Cl2
Filter and Weigh Residue
500 mL CH2Cl2 Phase
Extract CH2Cl2 3 Times with 165 mL Water Adjusted to pH-12 with NaOH
Aqueous Phase (Acids)
CH2Cl2 Phase (Base/Neutral)
Acidify Water to pH-1 with HCl
Extract 3 Times with 165 mL CH2Cl2
CH2Cl2 Layer Label: Dilute Acid Fraction
Discard Aqueous Layer
Combine CF2Cl2 Layer with Other Dilute Acid Fractions of Same Sample
See Flow Diagram for Organic Analysis Figure 16
CH2Cl2 Layer Label: Dilute Base/Neutral Fraction
Combine with Other Dilute/Base Neutral Fractions of Same Sample
See Flow Diagram For Organic Analysis Figure 16

Figure B-5. Flow scheme for the preparation of organic liquids and by-products.

APPENDIX C

SUPPORTING ORGANIC DATA

TABLE C-1. PRODUCT GAS EXTRACTABLE ORGANIC LOADING AND MASS FLOW RATE SUMMARY

	Units	Wellman-Galusha (Ft. Snelling)	Foster Wheeler/ STOIC	Riley	Lurgi-type (Kosovo)	Chapman	Wellman-Galusha (Glen Gery)
Coal Feed Rate	g/sec	250	270	670	4400	300	220
Dry Gas Flow Rate	m^3/sec	0.55	1.0	2.2	5.6	0.87	1.2
Molecular Weight Dry Gas	g/Mol	23	23	23	22	25	24
Organics Concentration	g/m^3	16	4.0[a]	9.1	7.7[b]	2.4	0.007
Organics Mass Flow Rate	g/sec	8.6	4.2	20	44[b]	2.1	0.0009
Product Gas Organics/ Coal Feed	Kg/ton	34	16	30	10[b]	6.8	0.004

[a] The combined product gas has a large amount of organics removed by the ESP on the top gas line. Loading in the dirty top gas is 12.6 g/SCM.

[b] The production rate of liquid by-products indicates that the organics concentration in the crude product gas could be as high as 35.7 g/m^3; the value shown is based on analysis of the vent gas from the LP coal lock and the flow rate of crude gas to Rectisol.

TABLE C-2. MASS CONCENTRATIONS OF LIGHT HYDROCARBONS IN CRUDE PRODUCT GAS[a]

	Wellman-Galusha (Ft. Snelling) Product Gas	Foster Wheeler/ STOIC Combined Product Gas	Riley Product Gas	Lurgi-type (Kosovo) Rectisol Feed	Chapman[b] Feeder Vent Gas	Wellman-Galusha (Glen Gery) Product Gas
Light Paraffins						
Ethane	7.8	17	6.1	57	84	0.01
Ethylene	3.6	2.9	3.0	4.6	NA[c]	NA
Propane	8.1	13	4.0	35	33	0.05
Butanes	4.6	7.8	8.5	17	22	ND[d]
Pentanes	6.0	6.2	NA	13	27	ND
Hexanes	6.9	8.8	NA	22	27	ND
Light Aromatics						
Benzene	>0.13	2.4	2.6	26	NA	ND
Toluene	.00	4.3	1.6	9.4	NA	ND
Xylene	.00	3.0	1.6	4.7	NA	ND
Total Conc., (ug/m^3 x 10^{-5})	37	65[b]	27	190	180	0.06
Gas flow rate, m^3/sec	0.55	1.0	2.2	5.6	0.87	1.2
Light hydrocarbons/g/sec	2.0	6.9	6.1	107	16	.074
Coal feed rate/g/sec	250	270	670	4490	300[b]	220
mg light hydrocarbons/g	8.1	24	9.0	24	52	0.034

[a] All values presented x10^{-5} ug/m^3; i.e., ethane concentration in Ft. Snelling product gas is 7.8 x 10^5 ug/m^3.

[b] Value based on the output from 2 gasifiers feeding a common train.

[c] NA = not analyzed.

[d] ND = not detected.

TABLE C-3. IDENTIFIED SPECIES IN EXTRACTED ORGANICS FROM GAS LIQUORS[a]

	Aqueous Process Condensate		
Compound	Kosovo	Chapman	Coke Oven
Phenols:			
Phenol	1,740 ± 100	1,460 ± 170	888 ± 52
o-Cresol	406 ± 27	420 ± 54	70.0 ± 2.3
m&p-Cresol	1,040 ± 60	1,120 ± 120	279 ± 14
2,6-Dimethylphenol	33.1 ± 10.0	19.1 ± 0.2	2.2 ± 1.0
2,4-Dimethylphenol	172 ± 17	196 ± 27	14.5 ± 0.1
3,5-Dimethylphenol	266 ± 21	172 ± 24	23.4 ± 0.8
3,4-Dimethylphenol	271 ± 24	681 ± 82	41.5 ± 1.3
1&2-Naphthol	13.0 ± 30.6	14.5 ± 0.3	4.5
p-Phenylphenol	<0.01	<0.01	<0.01
Total Phenols	3,940	4,080	1,320
Nitrogen Heterocyclics (Pyridines)[b]:			
Pyridine	12	2	11
2-Methylpyridine	19	5	11
3-Methylpyridine	45	11	12
Ethyl/Dimethylpyridines	7	1	1
Trimethyl/Ethylmethylpyridines	27	17	28
C_4-Pyridines	18	17	14
Quinoline	9	10	30
Total Pyridines	140	63	80
Total Phenols + Pyridines	4,080	4,140	1,400
Total Extractable Organic Carbon	4,600	7,600	5,680
Ratio (Phenols + Pyridines)/TCO	0.89	0.55	0.25

[a] All concentrations in mg/L; ± values indicate SD for 3 replicates.
[b] All components quantified as pyridine.

TABLE C-4. DETAILED ANALYSES OF ORGANICS FROM THE FOSTER-WHEELER/ STOIC GASIFIER[a]

RETENTION TIME	COMPOUND	PRODUCT GAS CONC.	ESP OIL CONC.	GAS ASH CONC.	CYCLONE DUST CONC.	ASH WATER CONC.	GAS COMBUST. EMISSION	OIL COMBUST. EMISSION
3.57	NI	0	0	0	3.45	0	0	0
4.17	CHLORINE COMPOUND	0	0	0	0.247	0	0	0
4.82	TOLUENE	0	0	0	0.454	0	0	0
6.5	NI	0	0	0	0.057	0	0	0
6.65	XYLENE	0	0	0	0.28	0	0	0
7.12	NI	0	0	0	0.103	0	0	0
7.27	NI	0	0	0	0.084	0	0	0
7.47	NI	0	0	0	0.082	0	0	0
8	NI	0	0	0	0.069	0	0	0
8.1	NI	0	0	0.151	0	0	0	0
8.15	NI	1517	0	0.249	0	0	0	0
8.23	NI	0	0	0.157	0	0	0	0
8.3	TRICHLOROPROPANE	0	0	0	0	0	0	10.5
8.3	NI	809	0	0	0	0	0	0
8.33	NI	0	0	0.086	0	0	0	0
8.43	ALKYL BENZENE	2731	0	0.555	0	0	0	0
8.45	NI	0	0	0	0.063	0	0	0
8.62	BENZALDEHYDE	0	0	0	0	0	8.43	3.81
8.63	ALKYL BENZENE	0	0	1.6	0	0	0	0
8.65	ALKYL BENZENE	8345	0	0	0	0	0	0
8.65	NI	0	0	0	0.054	0	0	0
8.78	ALKYL BENZENE	4147	0	0	0	0	0	0
8.78	PHENOL	0	0	0	0	3.23	0	0
8.78	NI	0	0	0.111	0	0	0	0
8.8	NI	0	0	0	0.033	0	0	0
8.93	NI	0	0	0.054	0	0	0	0
9.05	ALKYL BENZENE	0	0	0.243	0	0	0	0
9.07	ALKYL BENZENE	3287	0	0	0	0	0	0
9.1	m-MENTHANE	0	0	0.211	0	0	0	0
9.12	NI	1568	0	0	0	0	0	0
9.17	NI	0	0	0.107	0	0	0	0
9.17	NI	0	0	0	0.033	0	0	0
9.27	NI	0	0	0.048	0	0	0	0
9.37	ALKYL BENZENE	0	0	0.85	0.154	0	0	0
9.42	PHENOL	18600	0	0	0	0	0	0
9.48	NI	2023	0	0	0	0	0	0
9.52	n-C10 (174 c)	0	0	0	0.15	0	0	0
9.52	PHENOL	0	0	0	0	0	2.99	0
9.55	n-C10 (174 c)	0	0	1.05	0	0	0	0
9.58	n-C10 (174 c)	4248	0	0	0	0	0	0
9.62	NI	0	0	0	0	5	0	0
9.7	DECALIN	1113	0	0	0	0	0	0
9.72	NI	0	0	0.039	0	0	0	0
9.78	NI	0	0	0.049	0	0	0	0
9.83	NI	0	0	0.074	0	0	0	0

(continued)

TABLE C-4. (Continued)

RETENTION TIME	COMPOUND	PRODUCT GAS CONC.	ESP OIL CONC.	GAS ASH CONC.	CYCLONE DUST CONC.	ASH WATER CONC.	GAS COMBUST. EMISSION	OIL COMBUST. EMISSION
9.88	DECENE	1618	0	0	0	0	0	0
9.93	NI	0	0	0	0	4.63	0	0
9.98	NI	0	0	0.0226	0	0	0	0
10.07	NI	0	0	0	0.094	0	0	0
10.1	HYDROCARBON	0	0	0.621	0	0	0	0
10.12	NI	0	0	0	0	3.15	0	0
10.12	ALKYL BENZENE	10400	0	0	0	0	0	0
10.22	CYCLIC HYDROCARBON	0	0	0.376	0	0	0	0
10.27	NI	0	0	0.205	0	0	0	0
10.32	ALKANE	0	0	0.053	0	0	0	0
10.35	3,5-DIHYDROXYTOLUENE	0	0	0	0.442	0	0	0
10.42	INDANE	5259	0	0	0	0	0	0
10.43	ALKANE	0	0	0.187	0	0	0	0
10.53	C11 ALKENE	0	0	0.016	0	0	0	0
10.58	CHLORINATED ALKANE	0	0	0	8.82	0	0	0
10.6	C11 ALKENE	0	0	0.028	0	0	0	0
10.62	NI	2073	0	0	0	0	0	0
10.73	C4-ALKYL BENZENE	0	0	0	0	0	0	3.38
10.75	NI	0	0	0	0	3.1	2.09	0
10.77	NI	0	0	0.279	0	0	0	0
10.78	ALKYL BENZENE	2832	0	0	0	0	0	0
10.8	ALKYL BENZENE	0	0	0.049	0	0	0	0
10.88	C4-ALKYL BENZENE	0	0	0	0	0	0	2.09
10.9	NI	0	0	0	0	0	1.87	0
10.9	ALKANE	0	0	0.281	0	0	0	0
10.92	NI	1568	0	0	0	0	0	0
10.95	ALKYL BENZENE	0	0	0.153	0	0	0	0
10.98	CRESOL	8395	0	0	0	0	0	0
11.07	ALKANE	0	0	0.235	0	0	0	0
11.07	ALKYL BENZENE	4754	0	0	0	0	0	0
11.15	ALKYL BENZENE	0	0	0.042	0	0	0	0
11.17	C4-ALKYL BENZENE	0	0	0	0	0	0	3.33
11.18	NI	101	0	0	0	0	0	0
11.2	ALKANE	0	0	0.165	0	0	0	0
11.3	UNSATURATED HYDROCARBON	0	0	0.039	0	0	0	0
11.33	NI	0	0	0.062	0	0	0	0
11.35	NI	657	0	0	0	0	0	0
11.4	ALKYL BENZENE	0	0	0.111	0	0	0	0
11.4	CRESOL	0	270	0	0	0	0	0
11.43	ALKYL BENZENE	0	0	0.089	0	0	0	0
11.5	NI	4349	0	0	0	0	0	0
11.55	NI	0	0	0.067	0	0	0	0
11.6	ALKYL BENZENE	0	0	0.203	0	0	0	0
11.62	METHYLINDAN	0	0	0	0	0	0	15.9
11.63	ETHYL STYRENE	0	0	0	0	0	12.1	0

(continued)

TABLE C-4. (Continued)

RETENTION TIME	COMPOUND	PRODUCT GAS CONC.	ESP OIL CONC.	GAS ASH CONC.	CYCLONE DUST CONC.	ASH WATER CONC.	GAS COMBUST. EMISSION	OIL COMBUST. EMISSION
11.67	CRESOL	20300	0	0	0	0	0	0
11.8	NI	0	0	0	0	0	4.33	0
11.8	METHYLINDAN	0	0	0	0	0	0	4.99
11.87	NI	0	0	0.089	0	0	0	0
11.87	METHYL BENZOATE	0	0	0	0	4.66	0	0
11.88	NI	0	0	0	0.054	0	3.82	0
11.9	METHYL BENZOATE	0	0	0	0	0	0	7.19
11.93	n-C11 (196 c)	0	96	0	0	0	0	0
11.95	NI	0	0	0	0.181	0	0	0
11.95	n-C11 (196 c)	0	0	0	0	0	2.99	0
11.97	n-C11 (196 c)	0	0	0.979	0	0	0	0
12.05	n-C11 (196 c)	7333	0	0	0	0	0	0
12.08	ALKYL BENZENE	0	0	0.052	0	0	0	0
12.13	ALKYL BENZENE	2377	0	0	0	0	0	0
12.18	NI	0	0	0.067	0	0	0	0
12.27	XYLENOL	5512	0	0	0	0	0	0
12.35	ALKYL BENZENE	0	0	0.151	0	0	0	0
12.38	DIMETHYLINDAN	0	0	0	0	0	5.41	0
12.38	C2 ALKYL STYRENE	0	0	0	0	0	0	3.14
12.42	ALKYL BENZENE	2124	0	0	0	0	0	0
12.45	ALKYL BENZENE	0	0	0.036	0	0	0	0
12.55	ALKYL BENZENE	2174	0	0	0	0	0	0
12.6	HYDROCARBON	0	0	0.151	0	0	0	0
12.63	NI	506	0	0	0	0	0	0
12.63	DICHLOROPHENOL	0	0	0	0	11.9	0	0
12.8	CYCLIC C11	0	0	0.115	0	0	0	0
12.9	HYDROCARBON	0	0	0.086	0	0	0	0
13	NI	0	0	0	0	0	0	3.24
13	METHYL INDAN	3337	0	0	0	0	0	0
13.08	ALKYL BENZENE	0	0	0.016	0	0	0	0
13.12	NI	1213	0	0	0	4.1	0	0
13.2	METHYL CRESOL	0	28.9	0	0	0	0	0
13.25	NI	0	0	0.089	0	0	0	0
13.27	NI	3438	0	0	0	0	0	0
13.32	NI	0	0	0.101	0	0	0	0
13.33	XYLENOL	10000	0	0	0	0	0	0
13.4	NI	9254	0	0	0	0	0	0
13.52	ALKANE	0	0	0.019	0	0	0	0
13.57	NI	1668	0	0	0	0	2.24	0
13.57	ALIPHATIC ALDEHYDE	0	0	0	0	0	0	5.76
13.65	UNSATURATED HYDROCARBON	0	0	0.074	0	0	0	0
13.67	NI	354	0	0	0	0	0	0
13.68	METHYL CRESOL	0	241	0	0	0	0	0
13.75	NI	0	0	0	0	1.09	0	0
13.88	XYLENOL	7686	0	0	0	0	0	0

(continued)

TABLE C-4. (Continued)

RETENTION TIME	COMPOUND	PRODUCT GAS CONC.	ESP OIL CONC.	GAS ASH CONC.	CYCLONE DUST CONC.	ASH WATER CONC.	GAS COMBUST. EMISSION	OIL COMBUST. EMISSION
13.93	NI	0	0	0	0	0	2.16	0
13.95	NI	8344	0	0	0	0	0	0
14.03	NAPHTHALENE	0	125	0	0	0	0	0
14.05	NAPHTHALENE	0	0	0	0	0	0	29.3
14.06	NAPHTHALENE	0	0	0	0	0	21.6	0
14.07	NAPHTHALENE	0	0	0	0.111	0	0	0
14.08	NAPHTHALENE	6523	0	0	0	0	0	0
14.18	NI	0	0	0.039	0	3.55	0	0
14.2	ALKYL INDAN	2528	0	0	0	0	0	0
14.22	NI	0	0	0	0	0	1.83	0
14.27	NI	0	0	0.074	0	0	0	0
14.27	HYDROCARBON	3084	0	0	0	0	0	0
14.33	NI	2427	0	0	0	0	0	0
14.4	n-C12 (216 c)	0	222	0.348	0	0	0	0
14.42	NI	0	0	0	0.108	0	0	0
14.47	ALKYL INDAN	11833	0	0	0	0	0	0
14.53	NI	0	0	0	0	1.03	0	0
14.6	n-C12 (216 c)	1921	0	0	0	0	0	0
14.67	ALKYL PHENOL	1769	0	0	0	0	0	0
14.72	HYDROCARBON	0	0	0.076	0	0	0	0
14.72	NI	505	0	0	0	0	0	0
14.73	NI	0	77	0	0	1.72	0	0
14.82	HYDROCARBON	3590	0	0	0	0	0	0
14.9	MO	3944	0	0	0	0	0	0
15.03	NI	252	0	0	0	0	0	0
15.13	NI	0	0	0	0	5	0	0
15.23	NI	2730	0	0	0	0	0	0
15.3	ALKYL PHENOL	9507	0	0	0	0	0	0
15.33	NI	0	0	0.028	0	0	0	0
15.35	NI	0	0	0	0	2.01	0	0
15.5	ALKYL PHENOL	4247	0	0	0	0	0	0
15.58	ALKYL PHENOL	3289	0	0	0	0	0	0
15.7	METHYL TETRALIN	1365	0	0	0	0	0	0
15.8	ALKYL INDAN	1415	0	0	0	0	0	0
15.8	NI	0	0	0.016	0	0	0	0
15.88	NI	0	67.4	0	0	0	0	0
15.96	ALKYL INDAN	4045	0	0	0	0	0	0
16.03	NI	0	0	0.072	0	0	0	0
16.05	ALKYL PHENOL	6372	0	0	0	0	0	0
16.18	ALKYL PHENOL	6321	0	0	0	0	0	0
16.28	METHYL TETRALIN	2730	0	0	0	0	0	0
16.42	DIMETHYL INDAN	0	164	0	0	0	0	0
16.48	NI	7130	0	0	0	0	0	0
16.58	NI	0	86.7	0	0	0	0	0
16.6	NI	1011	0	0	0	0	0	0

(continued)

TABLE C-4. (Continued)

RETENTION TIME	COMPOUND	PRODUCT GAS CONC.	ESP OIL CONC.	GAS ASH CONC.	CYCLONE DUST CONC.	ASH WATER CONC.	GAS COMBUST. EMISSION	OIL COMBUST. EMISSION
16.67	NI	0	0	0.018	0	0	0	0
16.67	n-C13 (234 c)	5613	0	0	0	0	0	0
16.68	1-METHYLNAPHTHALENE	0	530	0	0	0	0	0
16.72	METHYL NAPHTHALENE	0	0	0	0	0	1.04	0
16.78	n-C13 (234 c)	0	491	0.734	0	0	0	0
16.8	ALKYL NAPHTHALENE	0	0	0	0.096	0	0	0
16.82	METHYL NAPHTHALENE	12591	0	0	0	0	0	0
16.9	NI	5663	0	0	0	0	0	0
16.98	NI	4045	0	0	0	0	0	0
17.1	NI	0	0	0	0	7.28	0	0
17.1	2-METHYLNAPHTHALENE	0	395	0	0	0	0	0
17.12	NI	0	0	0	0	0	2.12	0
17.18	NI	0	0	0	0	4.24	0	0
17.2	METHYL NAPHTHALENE	11226	0	0	0	0	0	0
17.28	AROMATIC COMPOUND	0	0	0.068	0	0	0	0
17.3	C3-ALKYL INDAN	0	125	0	0	0	0	0
17.38	ALKYL TETRALIN	7737	0	0	0	0	0	0
17.38	AROMATIC COMPOUND	0	0	0.028	0	0	0	0
17.48	C3-ALKYL INDAN	0	144	0	0	0	0	0
17.57	ALKYL TETRALIN	4601	0	0	0	0	0	0
17.67	HYDROCARBON	0	0	0.044	0	0	0	0
17.7	NI	708	0	0	0	0	0	0
17.78	C3-ALKYL INDAN	0	77	0	0	0	0	0
17.78	AROMATIC COMPOUND	0	0	0.096	0	0	0	0
17.85	ALKYL TETRALIN	5916	0	0	0	0	0	0
17.93	NI	1618	0	0	0	0	0	0
18.02	AROMATIC COMPOUND	0	0	0.038	0	0	0	0
18.05	NI	859	0	0	0	0	0	0
18.12	ALKYL BENZENE	0	0	0.072	0	0	0	0
18.27	ALKYL BENZENE	0	0	0.189	0	0	0	0
18.27	NI	0	77	0	0	0	0	0
18.28	HYDROCARBON	4500	0	0	0	0	0	0
18.28	NI	0	0	0	0	1.03	0	0
18.4	ALKYL BENZENE	0	0	0.195	0	0	0	0
18.43	NI	4298	0	0	0	0	0	0
18.53	HYDROCARBON	0	0	0.089	0	0	0	0
18.55	NI	0	250	0	0	0	0	0
18.6	ALKYL TETRALIN	5461	0	0	0	0	0	0
18.68	BIPHENYL	0	0	0	0	0	0	3.86
18.7	NI	0	0	0	0	0	1.64	0
18.73	NI	657	0	0	0	0	0	0
18.87	NI	0	0	0.018	0	0	0	0
18.88	NI	0	154	0	0	0	0	0
18.95	NI	3590	0	0	0	0	0	0
18.97	DIMETHYLNAPHTHALENE	0	241	0	0	0	0	0

(continued)

TABLE C-4. (Continued)

RETENTION TIME	COMPOUND	PRODUCT GAS CONC.	ESP OIL CONC.	GAS ASH CONC.	CYCLONE DUST CONC.	ASH WATER CONC.	GAS COMBUST. EMISSION	OIL COMBUST. EMISSION
19.03	HYDROCARBON	3843	0	0	0	0	0	0
19.08	NI	0	0	0	0	0	1.73	0
19.08	DIALKYL NAPHTHALENE	0	0	0	0.114	0	0	0
19.08	n-C14 (252 c)	0	790	0	0	0	0	0
19.1	n-C14 (252 c)	0	0	1.26	0	0	0	0
19.12	NI	1011	0	0	0	0	0	0
19.23	DIMETHYLNAPHTHALENE	0	510	0	0	0	0	0
19.23	n-C14 (252 c)	202	0	0	0	0	0	0
19.33	NI	4450	0	0	0	0	0	0
19.47	NI	1416	0	0	0	0	0	0
19.48	AROMATIC COMPOUND	0	0	0.032	0	0	0	0
19.57	DIMETHYLNAPHTHALENE	0	500	0	0	0	0	0
19.63	NI	0	963	0	0	0	0	0
19.67	DIMETHYL NAPHTHALENE	6068	0	0	0	0	0	0
19.75	DIMETHYL NAPHTHALENE	10114	0	0	0	0	0	0
19.88	AROMATIC COMPOUND	0	0	0.052	0	0	0	0
19.95	NI	1820	0	0	0	0	0	0
20	DIMETHYLNAPHTHALENE	0	173	0	0	0	0	0
20.03	NI	0	0	0.211	0	0	0	0
20.07	DIMETHYL NAPHTHALENE	2730	202	0	0	0	0	0
20.15	AROMATIC COMPOUND	0	0	0.157	0	0	0	0
20.15	DIMETHYL NAPHTHALENE	1769	0	0	0	0	0	0
20.27	NI	859	0	0	0	0	0	0
20.3	AROMATIC COMPOUND	0	0	0.032	0	0	0	0
20.33	NI	455	0	0	0	0	0	0
20.35	DIMETHYLNAPHTHALENE	0	250	0	0	0	0	0
20.4	HYDROCARBON	0	0	0.096	0	0	0	0
20.4	DIMETHYL NAPHTHALENE	1365	0	0	0	0	0	0
20.43	ALKANE	0	472	0	0	0	0	0
20.48	HYDROCARBON	3742	0	0	0	0	0	0
20.55	AROMATIC COMPOUND	0	0	0.281	0	0	0	0
20.57	NI	0	193	0	0	0	0	0
20.62	NI	0	0	0.125	0	0	0	0
20.62	ALKYL BENZENE	1820	0	0	0	0	0	0
20.63	ALKYL BENZENE	0	0	0	0	12.5	0	0
20.65	NI	0	472	0	0	0	0	0
20.65	AROMATIC COMPOUND	0	0	0	0	0	9.48	0
20.67	NI	0	0	0	0	0	0	7.14
20.68	AROMATIC COMPOUND	0	0	0.32	0	0	0	0
20.73	ALKYL BENZENE	1466	0	0	0	0	0	0
20.85	NI	960	0	0	0	0	0	0
21.02	?DIOCTYLETHANE	0	510	0	0	0	0	0
21.05	NI	6169	0	0	0	0	0	0
21.08	AROMATIC COMPOUND	0	963	0	0	0	0	0
21.1	DIALKYL NAPHTHALENE	0	0	0	0.046	0	0	0

(continued)

TABLE C-4. (Continued)

RETENTION TIME	COMPOUND	PRODUCT GAS CONC.	ESP OIL CONC.	GAS ASH CONC.	CYCLONE DUST CONC.	ASH WATER CONC.	GAS COMBUST. EMISSION	OIL COMBUST. EMISSION
21.12	NI	7737	0	0	0	0	0	0
21.17	HYDROCARBON	0	135	0	0	0	0	0
21.22	HYDROCARBON	0	0	0.402	0	0	0	0
21.22	ALKYL PHENOL	151	0	0	0	0	0	0
21.25	NI	0	1350	0	0.151	2.04	1.61	0
21.3	n-C15 (270 c)	6978	0	0	0	0	0	0
21.35	NI	0	96.3	0	0	0	0	0
21.4	NI	1314	0	0	0	0	0	0
21.58	NI	1163	28.5	0	0	0	0	0
21.6	NI	0	0	0	0	2.86	0	0
21.65	DIBENZOFURAN	0	135	0	0	0	0	0
21.7	DIBENZOFURAN	1466	0	0	0	0	0	0
21.77	NI	0	0	0	0.06	0	0	0
21.78	C5-ALKYL INDAN	0	732	0	0	0	0	0
21.83	NI	5158	0	0	0	0	0	0
21.87	C2-ALKYL NAPHTHALENE	0	318	0	0	0	0	0
21.9	ALKYL NAPHTHALENE	2124	0	0	0	0	0	0
21.97	C2-ALKYL NAPHTHALENE	0	289	0	0	0	0	0
22.02	ALKYL NAPHTHALENE	2023	0	0	0	0	0	0
22.03	AROMATIC COMPOUND	0	0	0.221	0	0	0	0
22.17	NI	50	0	0	0	0	0	0
22.17	C5-ALKYL INDAN	0	193	0	0	0	0	0
22.23	NI	0	0	0.135	0	0	0	0
22.3	C3-ALKYL NAPHTHALENE	0	173	0	0	0	0	0
22.35	ALKYL NAPHTHALENE	2579	0	0	0	0	0	0
22.5	NI	0	135	0	0	0	0	0
22.6	NI	0	0	0.086	0	0	0	0
22.65	NI	0	1700	0	0	0	0	0
22.68	ALKYL NAPHTHALENE	9203	0	0	0	0	0	0
22.72	C3-ALKYL NAPHTHALENE	0	289	0	0	0	0	0
22.75	NI	3135	0	0	0	0	0	0
23.05	FLUORENE	0	289	0	0	0	0	0
23.08	FLUORENE	1921	0	0	0	0	0	0
23.18	C3-ALKYL NAPHTHALENE	0	2420	0	0	0	0	0
23.22	ALKYL NAPHTHALENE	9406	0	0	0	0	0	0
23.3	n-C16 (288 c)	0	1730	0	0	0	0	0
23.3	NI	0	0	0	0.031	5.88	0	0
23.33	PHTHALATE	0	0	0	0	0	4.9	0
23.33	NI	0	0	1.22	0	0	0	0
23.35	NI	6068	0	0	0	0	0	0
23.42	NI	2124	0	0	0	0	0	0
23.42	METHYLDIBENZOFURAN	0	270	0	0	0	0	0
23.57	NI	0	231	0	0	0	0	0
23.57	ALKYL NAPHTHALENE	1871	0	0	0	0	0	0
23.8	ALKYL BIPHENYL	0	0	0	0	0	0	3.67

(continued)

TABLE C-4. (Continued)

RETENTION TIME	COMPOUND	PRODUCT GAS CONC.	ESP OIL CONC.	GAS ASH CONC.	CYCLONE DUST CONC.	ASH WATER CONC.	GAS COMBUST. EMISSION	OIL COMBUST. EMISSION
23.82	NI	0	0	0	0	0	2.92	0
23.83	METHYL FLUORENE	1112	0	0	0	0	0	0
23.83	ALKYL NAPHTHALENE	0	270	0	0	0	0	0
23.97	NI	0	0	0.049	0	0	0	0
24.02	NI	0	0	0.131	0	0	0	0
24.1	NI	0	231	0	0	0	2.12	0
24.1	METHYL FLUORENE	809	0	0	0	0	0	0
24.22	NI	0	0	0.109	0	0	0	0
24.27	HYDROCARBON	3944	1180	0	0	0	0	0
24.27	NI	0	0	0	0.064	0	0	0
24.43	NI	0	299	0	0	0	0	0
24.53	NI	0	106	0	0	0	0	0
24.62	NI	0	0	0.086	0	0	0	0
24.8	ALKYL NAPHTHALENE	657	0	0	0	0	0	0
24.82	NI	0	289	0	0	0	0	0
24.95	NI	0	202	0	0.084	0	0	0
24.95	ALKYL NAPHTHALENE	1466	0	0	0	0	0	0
25.1	NI	3843	0	0	0	0	0	0
25.13	C4-ALKYL NAPHTHALENE	0	1000	0	0	0	0	0
25.13	UNSATURATED HYDROCARBON	0	0	0.338	0	0	0	0
25.15	UNSATURATED HYDROCARBON	0	0	0	0	44.5	0	0
25.17	NI	0	684	0	0.156	0	0	0
25.17	UNSATURATED HYDROCARBON	0	0	0	0	0	26.4	26
25.23	NI	0	0	0.064	0.141	0	0	0
25.27	HYDROCARBON	4601	0	0	0	0	0	0
25.28	n-C17 (303 c)	0	1590	0	0	0	0	0
25.33	NI	0	0	0.135	0	0	0	0
25.35	NI	0	0	0	0.136	0	0	0
25.37	HYDROCARBON	4298	0	0	0	0	0	0
25.4	ALKANE	0	2040	0	0	0	0	0
25.5	C4-ALKYL NAPHTHALENE	0	144	0	0	0	0	0
25.6	NI	0	164	0	0	0	0	0
25.7	NI	1213	462	0	0	0	0	0
25.83	HYDROCARBON	3337	0	0	0	0	0	0
25.83	NI	0	0	0.072	0	0	0	0
25.87	C19 ALKENE	0	1880	0	0	0	0	0
25.93	NI	0	0	0.062	0	0	0	0
26.03	NI	4450	0	0	0	0	0	0
26.05	C11 ALKENE	0	2330	0	0	0	0	0
26.15	NI	0	0	0.054	0	0	0	0
26.22	ALKYL NAPHTHALENE	0	164	0	0	0	0	0
26.38	NI	0	38.5	0	0	0	0	0
26.55	NI	0	0	0.049	0	0	0	0
26.7	NI	0	86.7	0	0	0	0	0
26.78	NI	0	96.3	0	0	0	0	0

(continued)

TABLE C-4. (Continued)

RETENTION TIME	COMPOUND	PRODUCT GAS CONC.	ESP OIL CONC.	GAS ASH CONC.	CYCLONE DUST CONC.	ASH WATER CONC.	GAS COMBUST. EMISSION	OIL COMBUST. EMISSION
26.87	PHENANTHRENE	0	0	0	0	0	0	3.05
26.88	PHENANTHRENE	0	0	0	0	0	2.12	0
26.9	PHENANTHRENE	0	270	0	0	0	0	0
26.97	d10 ANTHRACENE	0	0	0	0	0	0	0
26.97	d10 ANTHRACENE	0	0	0	0	0	0	0
26.98	d10 ANTHRACENE	0	0	0	0	0	0	0
26.98	ANTHRACENE	3135	0	0	0	0	0	0
27	d10 ANTHRACENE	0	0	0	0	0	0	0
27	d10 ANTHRACENE	0	0	0	0	0	0	0
27	d10 ANTHRACENE	0	0	0	0	0	0	0
27.08	d10 ANTHRACENE	0	0	0	0	0	0	0
27.1	NI	0	0	0	0.234	0	0	0
27.13	n-C18 (317 c)	0	2450	0	0	0	0	0
27.2	NI	0	202	0	0	0	0	0
27.23	NI	0	0	0.049	0	0	0	0
27.28	NI	0	270	0	0	0	0	0
27.45	NI	0	116	0	0	0	0	0
27.73	NI	0	222	0	0	0	0	0
27.95	NI	0	183	0	0	0	0	0
28.22	NI	0	164	0	0	0	0	0
28.52	NI	0	38.5	0	0	0	0	0
28.65	NI	0	57.8	0	0	0	0	0
28.7	NI	0	231	0	0	0	0	0
28.78	NI	0	693	0	0	0	0	0
28.85	NI	0	0	0.029	0	0	0	0
28.87	NI	0	0	0	0.234	0	1.62	0
28.92	n-C19 (330 c)	0	2420	0	0	0	0	0
28.95	n-C19 (330 c)	1668	0	0	0	0	0	0
29.2	NI	0	376	0	0	0	0	0
29.32	NI	0	144	0	0	0	0	0
29.63	NI	0	67.4	0	0	0	0	0
29.85	NI	0	125	0	0	0	0	0
29.95	NI	0	77	0	0	0	0	0
30.05	NI	0	0	0	0	0.74	0	0
30.07	NI	0	0	0	0	0	1.76	0
30.3	NI	0	193	0	0	0	0	0
30.48	NI	0	491	0	0	0	0	0
30.5	NI	0	0	0	0.06	0	0	0
30.53	n-C20 (343 c)	960	0	0	0	0	0	0
30.55	NI	0	0	0.029	0	0	1.64	0
30.57	NI	0	0	0	0.285	0	0	0
30.62	n-C20 (343 c)	0	2860	0	0	0	0	0
30.65	NI	859	0	0	0	0	0	0
30.67	NI	0	0	0	0.181	0	0	0
30.72	NI	0	1200	0	0	0	0	0

(continued)

TABLE C-4. (Continued)

RETENTION TIME	COMPOUND	PRODUCT GAS CONC.	ESP OIL CONC.	GAS ASH CONC.	CYCLONE DUST CONC.	ASH WATER CONC.	GAS COMBUST. EMISSION	OIL COMBUST. EMISSION
30.88	NI	0	299	0	0	0	0	0
31.22	NI	0	86.7	0	0	0	0	0
31.4	NI	0	0	0	0.907	0	0	0
31.42	NI	0	135	0.161	0	0	0	0
31.42	SULFUR	0	0	0	0	29.8	0	0
31.52	NI	0	135	0	0	0	0	0
31.53	NI	0	0	0	1.44	0	0	0
31.92	NI	0	135	0	0	0	0	0
32.12	NI	0	1670	0	0	0	0	0
32.15	NI	0	0	0.032	0	0	0	0
32.15	n-C21 (356 c)	0	0	0	0.267	0	0	0
32.17	n-C21 (356 c)	657	0	0	0	0	0	3.24
32.23	n-C21 (356 c)	0	4080	0	0	0	0	0
32.4	NI	0	0	0	0	1.77	0	0
32.52	NI	0	231	0	0	0	0	0
32.72	NI	0	48.2	0	0	0	0	0
33.1	NI	0	57.8	0	0	0	0	0
33.25	NI	0	116	0	0	0	0	0
33.32	NI	0	86.7	0	0	0	0	0
33.68	C22 ALKENE	0	1440	0	0	0	0	0
33.7	n-C22 (368 c)	0	0	0	0.343	0	0	0
33.72	NI	0	0	0.032	0	0	0	0
33.72	n-C22 (368 c)	556	0	0	0	0	0	8.86
33.73	NI	0	0	0	0	0.69	1.33	0
33.8	n-C22 (368 c)	0	4690	0	0	0	0	0
34.07	NI	0	260	0	0	0	0	0
34.22	NI	0	144	0	0	0	0	0
34.6	NI	0	125	0	0	0	0	0
34.68	NI	0	38.5	0	0	0	0	0
35.17	C23 ALKENE	0	1410	0	0	0	0	0
35.18	n-C23 (380 c)	556	0	0	0.369	0	0	0
35.2	NI	0	0	0.034	0	0	1.52	0
35.2	n-C23 (380 c)	0	0	0	0	0	0	14.2
35.28	n-C23 (380 c)	0	4690	0	0	0	0	0
35.55	NI	0	347	0	0	0	0	0
36.15	NI	0	96.3	0	0	0	0	0
36.6	C24 ALKENE	0	1050	0	0	0	0	0
36.6	n-C24 (391 c)	0	0	0	0.397	0	0	0
36.63	NI	0	0	0.039	0	0	0	0
36.7	DIOCTYL ADIPATE	0	0	0	0	11.8	0	0
36.7	Di-n-OCTYL ADIPATE	5006	0	0	0	0	6.48	0
36.72	n-C24 (391 c)	0	5010	0	0	0	0	0
36.77	Di-n-OCTYL ADIPATE	0	0	0	0	0	0	241
36.98	NI	0	222	0	0	0	0	0
37.52	NI	0	212	0	0	0	0	0

(continued)

TABLE C-4. (Continued)

RETENTION TIME	COMPOUND	PRODUCT GAS CONC.	ESP OIL CONC.	GAS ASH CONC.	CYCLONE DUST CONC.	ASH WATER CONC.	GAS COMBUST. EMISSION	OIL COMBUST. EMISSION
37.98	n-C25 (401 c)	0	0	0	0.514	0	0	0
38	n-C25 (401 c)	0	0	0	0	0	0	14.7
38	NI	0	0	0.038	0	0	0	0
38.1	n-C25 (401 c)	0	5210	0	0	0	0	0
38.33	NI	0	202	0	0	0	0	0
38.72	NI	0	0	0	0.13	0	0	0
38.73	NI	0	0	0.064	0	0	0	0
38.77	bis(2-ETHYLHEXYL) PHTHALATE	0	0	0	0	7.92	0	20.9
38.77	n-C25 (401 c)	1011	0	0	0	0	0	0
38.78	NI	0	28.9	0	0	0	0	0
38.78	bis(2-ETHYLHEXYL) PHTHALATE	0	0	0	0	0	5.42	0
39.2	NI	0	231	0	0	0	0	0
39.3	n-C26 (412 c)	0	0	0	0.373	0	0	0
39.33	n-C26 (412 c)	0	0	0	0	0	0	11.7
39.4	NI	0	4710	0	0	0	0	0
39.67	NI	0	86.7	0	0	0	0	0
40.18	NI	0	67.4	0	0	0	0	0
40.58	n-C27 (422 c)	0	0	0	0.285	0	0	0
40.62	n-C27 (422 c)	0	0	0	0	0	0	5.95
40.68	n-C27 (422 c)	0	3940	0	0	0	0	0
40.95	NI	0	135	0	0	0	0	0
41.82	NI	0	0	0	0.168	0	0	0
41.9	n-C28 (432 c)	0	2270	0	0	0	0	0
43	NI	0	0	0	0.049	0	0	0
43.08	n-C29 (441 c)	0	1770	0	0	0	0	0
43.48	NI	0	48.2	0	0	0	0	0
43.62	NI	0	212	0	0	0	0	0
44.05	NI	0	144	0	0	0	0	0
44.18	NI	0	0	0	0	1.99	0	0
44.22	NI	0	626	0	0	0	0	0
45.1	NI	0	0	0	0.06	0	0	0
45.18	NI	0	356	0	0	0	0	0
45.33	NI	0	327	0	0	0	0	0
45.77	NI	0	356	0	0	0	0	0
46.22	NI	0	173	0	0	0	0	0
46.87	NI	0	125	0	0	0	0	0

a All concentrations are in ug/m3

b NI = Not identified

c Estimated molecular weight

TABLE C-5. POLYAROMATIC AMINES IN ESP OIL FROM THE FOSTER-WHEELER/STOIC GASIFIER AS DETERMINED BY GC-MS (14)

Component	Concentration (ug/g)
1-Aminonaphthalene	9
2-Aminonaphthalene	30
C_1-Aminonaphthalenes	4-24[a]
C_2-Aminonaphthalenes	7-10[b]
C_3-Aminonaphthalene	7
Aminofluorene	9
1-Aminoanthracene	13
2-Aminoanthracene	2
C_1-Aminoanthracene	1
Acridine	26

[a] Range of results for five isomers.
[b] Range of results for three isomers.

TABLE C-6. CONCENTRATION OF PRIORITY POLLUTANTS IDENTIFIED IN PRODUCT AND DISCHARGE STREAMS: FOSTER-WHEELER/STOIC GASIFIER

Compound	Gasifier Ash (ug/g)	Ash Pan Water (ug/L)	Cyclone Dust (ug/g)	ESP Oil to Boiler #3 (ug/g)	Combined Product Gas (ug/Nm^3)	Emissions from Product Gas Combustion (ug/Nm^3)	Emissions from ESP Oil Combustion (ug/Nm^3)
Phenol	ND[a]	3.3	ND	2400	4200	3.7	30
2,4-dimethylphenol	ND	ND	ND	ND	2.4E4	ND	ND
Naphthalene	0.01	0.33	0.15	310	7800	9.4	16
1-methylnaphthalene	ND	ND	0.01	540	7500	1.4	1.8
2-methylnaphthalene	ND	ND	0.01	370	6300	1.2	1.7
Dimethylnaphthalene	ND	ND	0.05	2500	2.3E4	1.4	1.3
Phenanthrene	ND	ND	0.01	320	310	0.32	0.72
Anthracene	ND	ND	ND	240	220	ND	ND
Fluorene	ND	ND	ND	320	29	0.36	0.48
Pyrene	ND	ND	0.04	ND	120	0.14	0.46
Benzo(a)anthracene	ND	ND	ND	240	ND	ND	ND
Bis(2-ethylhexyl) phthalate[b]	0.04	6.7	ND	20	1200	5.0	20
Stream Flow Rate (per sec)	35g	9.1mL	0.2±0.1g	250g	0.95m^3	4.67m^3	4.17m^3

[a] ND = Not detected.
[b] Probable artifact of sample handling.

TABLE C-7. PHENOLIC SPECIES ISOLATED AS AN ACID FRACTION FROM KOSOVO ORGANICS

Component	Boiling Point °C	RT[a] (min)	Tar (mg/g)	Medium Oil (mg/g)	Heavy Tar (mg/g)	Phenolic Water (mg/L)
Phenol	182	8.55	5.9	19	3.3	0.69
o-cresol (as phenol)	191	9.50	4.9	19	2.4	0.26
m-cresol	202	9.70	13	38	6.7	0.61
p-cresol (as phenol)	202	9.90	1.4	3.1	0.70	0.10
2,6-dimethyl phenol	212	10.10	1.2	4.6	0.57	0.013
NI[b]		10.35	1.3	4.0	0.61	0.020
3,4-dimethyl phenol	225	10.50	7.5	22	3.6	0.13
NI		10.65	10	22	5.4	0.21
2,4-dimethyl phenol	237	10.95	3.9	12	2.0	0.19
NI		11.20	2.1	4.7	0.98	0.21
NI		11.30	3.7	8.3	1.7	0.020
NI		11.45	3.3	6.0	1.9	0.076
NI		11.0	2.8	5.0	1.4	0.010
NI		11.70	4.3	9.2	1.8	0.010
NI		12.35	2.6	3.4	1.2	——[c]
NI		12.40	2.7	6.1	1.2	0.052
1-Naphthol (as phenol)	288	13.20	1.0	0.73	0.69	NF[d]
Sum of Identified Peaks			38.8	15.43	19.96	1.993
Sum of Unidentified Listed Peaks			32.9	70.67	16.19	0.698
Sum of Other Peak Areas (as phenol)			94	42	81	0.21
Total Peak Area (as phenol)			165.7	228.1	117.15	2.901
% of Total Area Identified and Reported as phenol			23	51	17	69

[a] RT = Gas chromatographic retention time.

[b] NI = Not identified, quantified as phenol.

[c] — = No entry.

[d] NF = Not found.

TABLE C-8. CONCENTRATION OF ALKYL MERCAPTANS IN KOSOVO STREAMS (ppmv/v)

Gas Stream	CH_3SH	C_2H_5SH
Fleissner Autoclave Vent	3400	2100
Low Pressure Coal Lock Vent	420	220
High Pressure Coal Lock Vent	460	210
Start Up Vent	490	240
H_2S - Rich Waste Gas	2100	780
CO_2 - Rich Waste Gas	8.5	4.4
Crude Product Gas	590	200
Tar Tank Vent	390	240
Medium Oil Tank Vent	5200	2100
Tar Separation Waste Gas	2500	1600
Phenolic Water Tank Vent	2100	7200
Ammonia Stripper Vent	290	100
Naphthalene Storage Tank Vent	2600	9700
Waste Gases to Flare		

TABLE C-9. ALKYL MERCAPTANS IN HEAD SPACE OVER KOSOVO BY-PRODUCTS AND WASTES (ppmv/v)

Head Space	CH_3SH	C_2H_5SH
Tar	trace[a]	30
Medium Oil	9.7	1,199
Naphthalene	190	145,547
Heavy Tar	trace	2
Phenolic Water	3.2	128

[a] Trace means approximately 1 ppmv.

Conversion Factor:

$PPM \times F = mg/m^3$; $F_{CH_3SH} = 1965$; $F_{C_2H_5SH} = 1168$

TABLE C-10. THIOPHENES IN KOSOVO MEDIUM OIL[a]

Compound	Concentration[b]
Thiophene	160
2-methyl thiophene	660
3-methyl thiophene	540
2,5-dimethyl thiophene	210
Dimethyl or ethyl thiophene(s)	420
Dimethyl or ethyl thiophene(s)	390
Trimethyl or ethyl thiophene(s)	240
Trimethyl or ethyl thiophene(s)	280
Benzothiophene	340
Methyl benzothiophene	420
Total Thiophenes	3660

[a] Each entry represents a GC peak or cluster of peaks. Two lines bearing the same name indicate different compounds or different isomers of the same compound. E.g., 2,3-dimethyl thiophene, 2,4-dimethyl thiophene, 2,6-dimethyl thiophene, 2-ethyl thiophene, and 3-ethyl thiophene (see Figure 28).

[b] Approximate concentrations in ug/mL (based on response of thiophene).

TABLE C-11. NITROGEN HETEROCYCLICS IN SELECTED KOSOVO STREAMS[a]

Nitrogen-Bearing Compound	Phenolic[b] Water	Medium[c] Oil
Pyridine	28	5400
2-methyl pyridine	29	4200
3- & 4-methyl pyridine	13	2900
Dimethyl or ethyl pyridine(s)	39	2300
Dimethyl or ethyl pyridine(s)	7	2300
Alkyl pyridine(s)	16	990
Alkyl pyridine(s)	10	2600
Quinoline	5	710
C_1 Alkyl quinoline(s)	--[d]	720
C_2 Alkyl quinoline(s)	12	690
Total Nitrogen Heterocyclics	159	22,810

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[a] Each entry represents a GC peak or peak cluster. Duplicate entries indicate different compounds or different isomers of the same compound.
[b] Concentrations in mg/L based on GC-MS response factor for 3-nitrotoluene.
[c] Concentrations in mg/L based on GC-HECD response to pyridine.
[d] Not reported.

TABLE C-12. COMPOUND CLASSES IN AQUEOUS SAMPLES FROM THE KOPPERS-TOTZEK PROCESS[a]

Component	Rectisol Condensate		Settling Pond Effluent		Compressor Condensate		Input Water	
	1[b]	2	1	2	1	2	1	2
Aliphatic Hydrocarbons	10,190	48,130	5	0.009				
Phenols		480						
2-3 Ring Polycyclics	100	480			1,960	30		
4-3 Ring Polycyclics	100	480						
Fused Non-alternate Polycyclics		480						
Phthalate esters		480	5	0.009	190	310	560	880
Sulfur (S_8)	1,020	4,810			1,960	3,080		
Unsaturated Hydrocarbons				0.9				
Primary Alcohols			55				60	
Secondary Alcohols			55	9				
Ketones				0.09				
Unsaturated Alkyl halides			0.5					
Phenols						30		
Chlorinated Phenols					20	30		
Carboxylic Acids						30		
Esters					1,960			
Nitroaromatic Compounds							60	

[a] All concentrations in ug/L.

[b] 1. sampled 11/12 - Ref. 13.
2. sampled 11/19 - Ref. 13.

TABLE C-13. ORGANIC PRIORITY POLLUTANT SCREENING OF KOPPERS-TOTZEK AQUEOUS STREAMS[a]

Compound	Reused Condensate	Combined Compressor Condensate	Settling Pond Effluent	Input Water
Naphthalene	T[b]	T	-[c]	-
Fluorene	1.6	-	-	-
Acenaphthalene	T	-	-	-
Anthracene + Phenanthrene	4.6	-	-	-
Fluoranthene	6.3 - 19	-	-	-
Pyrene	25 - 97	-	-	-
Chrysene	34	-	-	-
Butyl Benzyl Phthalate[d]	T	T	T	-
Diethyl Phthalate[d]	T	T	-	-
Phenol	T	T	-	-
2,4-Dimethyl Phenol	T	-	-	-
Chloroform	T	-	T	-
Di-n-Butyl Phthalate[d]	-	6.0	-	-
Chloromethane	-	7.8	-	-
4-m-Cresol	-	2.3	-	-
Nitrobenzene	-	-	-	T
1,2,4-Trichlorobenzene	-	-	-	T
Isophrene	-	-	-	T
Bis-2-Ethylhexyl Phthalate[d]	-	-	-	T
Di-n-Octyl Phthalate[d]	-	-	-	T

[a] All concentrations in ug/L.
[b] T = Found at <1 ug/L.
[c] - = Not reported.
[d] Common artifacts of sampling and sample handling.

TABLE C-14. MAJOR LIGHT ORGANIC SPECIES IN BI-GAS PROCESS GAS STREAMS[a]

Component	Selexol Inlet Gas	Acid Gas	Selexol Outlet Gas
Toluene	1.0E4	2.6E5	9.0E1
C_2-Benzene	2.6E2	8.8E3	2.0E1
Styrene	2.7E2	2.0E4	9.0E0
Indan	3.1E2	1.7E4	2.0E0
Indene	2.9E2	1.3E5	4.0E0
Naphthalene	3.2E4	2.9E5	1.1E2
2-Methyl naphthalene	2.4E2	4.3E3	<2.0E0
1-Methyl naphthalene	1.5E2	2.2E3	<2.0E0
Biphenyl	3.2E2	2.3E3	<2.0E0

[a] All concentrations in ug/m^3.

TABLE C-15. SPECIATED ORGANICS FROM THE KRW PROCESS - BITUMINOUS COAL[a]

	Molecular Weight	Raw Product Gas (6/19/83)	Raw Product Gas (6/20/83)	Product Gas From PG Cooler (6/19/83)	Product Gas From RG Cooler[b] (6/20/83)	Product Gas From Radian Chiller Outlet (6/19/83)
Indene	116	2.4 E1	6.2 E1	5.7 E1	8.5 E1 4.7 E1	9.0 E1
Indan	118	6.3 E1	4.8 E1	1.9 E0	4.3 E1 3.4 E1	3.9 E1
Naphthalene	128	1.2 E2	1.3 E2	9.4 E0	7.3 E1 4.2 E1	8.9 E1
Unknown	134	NM[c]	NM	NM	2.2 E0 2.7 E0	NM
Unknown	134	NM	NM	NM	2.7 E0 2.7 E0	NM
Unknown	141	NM	NM	NM	NM	2.3 E0
C_{10} Hydrocarbon	142	NM	NM	NM	NM	1.1 E1
Methyl Naphthalene	142	2.3 E1	1.1 E1	1.1 E1	5.7 E0 5.7 E0	1.1 E1
Acenaphthalene	152	ND[d]	ND	4.9 E0	3.1 E0	1.2 E1
Acenaphthene	154	1.2 E1	7.4 E1	3.1 E1	3.0 E0 2.5 E0	1.2 E1
Biphenylene	152	NM	NM	4.9 E0	3.0 E0 3.7 E0	1.2 E1
Biphenyl	154	1.9 E0	1.2 E1	2.5 E0	1.2 E1 1.2 E0	2.5 E0
Dimethyl Naphthalene	156	NM	NM	NM	2.5 E0 2.5 E0	NM
C_2 Naphthalene	156	NM	NM	4.5 E0	NM	NM
C_{11} Alkane	156	NM	NM	NM	NM	3.7 E0
Fluorene	166	6.7 E-1	1.3 E1	2.7 E0	6.7 E-1	2.7 E0
Anthracene	178	ND	ND	ND	ND	ND
Phenanthrene	178	1.4 E0	2.1 E1	2.1 E0	1.4 E0	1.4 E0
Fluoranthene	202	8.1 E-1	5.8 E0	ND	1.6 E0	ND
Pyrene	202	1.6 E0	1.6 E0	ND	8.1 E-1	ND
Sulfur Compounds						
Benzothiophene	134	2.2 E1	3.3 E1	1.6 E1	1.1 E1 1.1 E1	2.2 E1
Trithiolane	138	NM	NM	NM	2.8 E0 2.8 E0	NM
Tetrathiocyclohexane	156	NM	NM	NM	NM	5.1 E0
Pentathiocyclohexane	174	2.8 E1	NM	1.4 E1	NM	4.3 E1
Dibenzothiophene	184	ND	ND	7.5 E-1	ND	ND
Pentathioheptene	188	NM	NM	1.5 E1	NM	NM
Pentathiocycloheptane	188	3.1 E1	2.3 E1	3.8 E1	2.3 E0 3.1 E0	6.9 E1
N Compounds						
Pyridine	79	6.5 E0	9.7 E1	7.4 E1	6.8 E1	6.5 E0
Aniline	93	1.5 E0	1.1 E0	ND	ND	ND
Benzonitrile	103	8.4 E0	8.4 E0	NM	NM	NM
Carbazole	167	ND	ND	ND	ND	ND
Oxygen Compounds						
Phenol	94	5.8 E4	8.8 E1	1.2 E1	7.7 E0	7.7 E0
Cresol	108	8.8 E3	ND	8.8 E0	1.3 E0	ND
Benzoic Acid	122	ND	ND	2.5 E2	3.7 E2 4.3 E2	ND
Indanone	132	NM	NM	NM	5.4 E-1 5.4 E-1	NM
Ethylbenzaldehyde	134	NM	NM	NM	1.1 E0 1.6 E0	NM
Methylbenzoate	136	NM	NM	5.6 E-1	2.2 E0 2.8 E0	
Dimethylacetophenone	148	NM	NM	NM	1.8 E0 1.8 E0	NM
Dibenzofuran	168	ND	6.9 E-1	D (Tr)[e]	6.9 E-1	ND
Sum ug/m^3		4.1 E2	6.4 E-1	5.6 E2	709.1	4.4 E2
Number of Components Detected		19	18	21	27	19

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[a] All concentrations in ug/m^3.
[b] Duplicate analysis results reported.
[c] NM = Not measured and not determined.
[d] ND = Not detected.
[e] D = Detected but not quantifiable.

TABLE C-16. SPECIATED ORGANICS FROM THE KRW PROCESS - SUBBITUMINOUS COAL[a]

	Molecular Weight	Raw Product Gas	PC Cooler Product Gas	RC Cooler Product Gas	Test Chiller
Indene	116	ND[b]	ND	1.4 E0[c]	1.1 E2
Indan	118	NM[d]	ND	4.8 E-1	2.8 E1
Naphthalene	128	1.6 E2	>7.3 E1	2.4 E1	8.4 E1
Tetralin	132	4.9 ED	D[e]	ND	ND
Methylnaphthalene	142	7.0 E0	2.9 E0	5.8 E-1	3.5 E0
Acenaphthalene	152	2.5 E0	3.7 E0	ND	1.9 E0
Biphenyl	154	7.6 E0	1.3 E0	ND	1.3 E0
Acenaphthene	154	1.9 E0	2.5 E0	D	2.5 E0
Fluorene	166	1.4 E1	2.0 E0	ND	2.0 E0
Anthracene	178	ND	D	ND	ND
Phenanthrene	178	2.9 E1	3.6 ED	7.3 E-1	3.6 E0
Fluoranthene	202	3.3 E0	D	ND	8.2 E-1
Pyrene	202	3.3 E0	ND	ND	1.7 E0
Cyclopentaphenanthrene		D	ND	ND	ND
Sulfur Compounds					
Benzothiophene	134	ND	ND	ND	ND
Trithiolane	138	NM	ND	ND	5.6 E-1
Tetrathiocyclohexane	156	ND	ND	1.3 E0	1.3 E0
Dibenzothiophene	184	3.8 E0	D	ND	ND
Pentathiocycloheptane	188	ND	ND	3.1 E0	ND
Nitrogen Compounds					
Pyridine	79	ND	NM	4.8 E1	9.7 E1
Aniline	93	ND	NM	ND	ND
Carbazole	167	1.4 E0	ND	ND	ND
Oxygen Compounds					
Phenol	94	ND	ND	ND	8.5 E0
Cresol	108	ND	ND	ND	ND
Benzoic Acid	122	ND	NM	2.5 E1	ND
Dibenzofuran	168	2.1 E0	6.9 E-1	ND	6.9 E-1
Sum		2.4 E2	9.0 E1	1.0 E2	3.5 E2
Number of Components		13	8	9	16

[a] All concentrations in ug/m^3.
[b] ND = not detected.
[c] 1.4E0 = 1.4 x 10^0.
[d] NM = not measured.
[e] D = at threshold of detection.

TABLE C-17. SPECIATED ORGANICS FROM THE KRW PROCESS - LIGNITE[a]

	Molecular Weight	Product Gases (ug/m^3)			
		Raw Gas	PG Cooler Gas	RG Cooler Gas	Test Cooler Gas
Indene	116	D[b]	9.5 E0	1.9 E1	4.7 E0
Indan	118	NM[c]	6.8 E1	2.5 E1	1.2 E1
C_3 Benzene	124	NM	NM	2.4 E1	NM
Naphthalene	128	9.4 E1	2.1 E2	4.7 E1	5.2 E0
Methylindene	130	NM	NM	1.3 E1	NM
Decane	142	NM	NM	1.1 E1	NM
Methyl naphthalene	142	2.9 E0	1.7 E0	5.8 E-1	5.8 E-1
Dimethyl Indene	144	NM	NM	9.4 E0	NM
Unknown	144	NM	NM	5.3 E0	NM
Unknown	150	NM	NM	NM	1.8 E0
Acenaphthalene	152	3.1 E0	ND[d]	ND	D
Acenaphthene	154	1.3 E1	D	3.1 E1	6.3 E-1
Biphenyl	154	3.1 E0	1.3 E0	D	D
C_{11} Alkane	156	NM	NM	1.2 E1	NM
Unknown	156	NM	1.1 E1	NM	NM
Unknown	156	NM	1.1 E1	NM	NM
Fluorene	166	1.4 E1	ND	D	ND
Anthracene	178	7.2 E-1	ND	ND	ND
Phenanthrene	178	3.6 E1	ND	7.2 E-1	D
Diphenylpropene	196	NM	NM	9.6 E0	NM
Hydrocarbon	200	NM	1.9 E1	NM	NM
Fluoranthene	202	2.5 E0	ND	D	ND
Pyrene	202	3.3 E0	ND	D	ND
C_{20} Alkane	262	NM	NM	NM	1.9 E1
C_{22} Alkene	286	NM	NM	3.5 E1	NM
Sulfur Compounds					
Benzothiophene	134	ND	1.1 E1	1.6 E0	1.6 E0
Tetrathiocyclohexene	156	2.6 E0	NM	1.8 E1	NM
Pentathiocyclohexane	174	NM	NM	NM	NM
Dibenzothiophane	184	ND	ND	ND	ND
Pentathiocycloheptene	188	NM	3.2 E1	NM	NM
Sulfur containing HC's	(188)	NM	NM	NM	4.8 E1
Nitrogen Compounds					
Pyridene	79	6.5 E0	2.3 E2	8.1 E1	6.5 E0
Anilene	93	1.5 E0	5.3 E1	ND	ND
Carbazole	167	ND	ND	ND	ND
Oxygen Compounds					
Phenol	94	NM	6.5 E1	ND	NM
Cresol	108	ND	ND	ND	ND
Benzoic Acid	122	ND	ND	7.0 E2	6.5 E2
Adipate	146	3.0 E1	NM	5.0 E1	NM
Phenylbutenone	146	NM	NM	4.8 E0	NM
Propylmethoxybenzene	150	NM	NM	9.2 E0	NM
Hydroxymethoxybenzaldehyde	152	1.2 E0	NM	NM	NM
Dibenzofuran	168	2.1 E0	ND	ND	D
Dioclyladipate	302	NM	NM	NM	8.9 E1
Alkylbenzylether	(302)	NM	NM	2.7 E1	NM
Sum		2.2 E2	6.2 E2	1.1 E2	8.4 E2
Number of Components Detected		16	13	22	12

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[a] All concentrations in ug/m^3.
[b] D = At threshold of detection.
[c] NM = Not measured.
[d] ND = Not detected.

TABLE C-18. ORGANICS IN PRODUCT GAS STREAMS OF THE KRW GASIFIER[a]

	Type of Coal		
Gas Stream	Bituminous	Subbituminous	Lignitic
Raw Product Gas[b]	4.1 E2[c]	2.4 E2	2.2 E2
Raw Product Gas[b]	6.4 E2[d]	NR[e]	NR
From PG Cooler	5.6 E2	9.0 E1	6.2 E2
From RG Cooler	7.1/6.8 E2[f]	1.0 E2	1.1 E3
From Test Cooler	4.4 E2	3.5 E2	8.4 E2

[a] Sum of organic concentrations as speciated by GC/MS (ug/m^3)

[b] Consists of recycled gas and product gas.

[c] Test 6/19/83.

[d] Test 6/20/83.

[e] NR = Not reported.

[f] Duplicate analyses.

TABLE C-19. KRW COAL GASIFIER PDU - ORGANICS IN AQUEOUS STREAMS USING WATER QUALITY PARAMETER MEASUREMENT METHODS[a]

Property	Type of Coal		
	Bituminous	Subbituminous	Lignitic
R12 Quench Recycle Water			
TOC	90 ± 2.1	77 ± 3.1	620 ± 690
COD	320 ± 61	220 ± 21	230 ± 130
Oil & Grease	18	10	2.7 ± 1.6
Phenol	9.9 ± 11	1.4 ± 1.7	ND (0.01)[b]
R15 Recycle Cooler Water			
TOC	19 ± 3.6	44 ± 6	2300 ± 2800
COD	150 ± 23	160 ± 78	59 ± 53
Oil & Grease	6 ± 9.5	2.8 ± 0.6	ND (1)
Phenol	ND (.005)	2.7 ± 1.4	ND (0.01)
R19 Separator Pit Water (Nearest to Discharge Water)			
TOC	54 ± 2.5	47 ± 1.4	110
COD	220 ± 15	150 ± 0	100
Oil & Grease	4.3 ± 5.0	3.4 ± 3.6	2
Phenol	ND (0.005)	0.048 ± 0.042	ND (0.01)
R30 Makeup Recycle Water			
TOC	47 ± 1.0	25 ± 16	1100 ± 590
COD	190 ± 100	69 ± 44	38 ± 1
Oil & Grease	6.3 ± 1.7	ND (1)	1.4 ± 0.8
Phenol	ND (0.005)	0.037 ± 0.032	ND (0.01)
R31 Diluted Flocculant			
TOC	NM[c]	620	NM
COD	NM	2400	NM
Oil & Grease	NM	ND (1)	NM
Phenol	NM	ND (0.02)	NM

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[a] Concentrations in mg/L.
[b] ND() = Not detected (detection limit).
[c] NM = Not measured.

TABLE C-20. KRW WASTEWATER ANALYSIS RESULTS - EXTRACTABLE ORGANICS (BITUMINOUS COAL TEST)[a]

			R-12 Quench Recycle		R-15 PG Cooler Recycle		R-19 Separator Pit Water	R-30 Recycle Water		R-32 Compressor Condensate
	MW[b]	LOC[c]	B/WH-522 6-19-83	B/WH-764 6-4-83	B/WH-521 6-19-83	B/WH-765 6-21-83	B/WH-766 6-21-83	B/WH-519 6-19-83	B/WH-767 6-21-83	B/WH-768 6-19-83
			DISSOLVED:	TOTAL:	DISSOLVED:	TOTAL:	TOTAL:	DISSOLVED:	TOTAL:	TOTAL:
Xylene	106	1	NM[d]	NM	NM	10	NM	NM	NM	NM
Indene	116	1	ND[e]	ND	NM	20	10	NM	ND	2
Indan	118	1	NM	NM	NM	NM	NM	NM	NM	NM
Naphthalene	128	1	ND	30	46	340	260	7	ND	90
Methylindene	130	2	ND	NM	NM	NM	NM	NM	NM	NM
Methylnaphthalene	142	1	ND	ND	ND	30	9	ND	ND	ND
Acenaphthylene	152	1	ND	1	ND	100	40	ND	ND	ND
Biphenyl	154	1	ND	0.2	ND	20	9	ND	ND	0.6
Acenaphthene	154	1	ND	1	ND	60	20	ND	ND	10
Fluorene	166	1	ND	1	ND	100	20	ND	ND	3
Anthracene	178	1	ND	ND	ND	100	3	ND	ND	ND
Phenanthrene	178	1	ND	3	ND	340	7	ND	ND	10
Acephenanthrylene	190	2	NM	ND	NM	20	ND	NM	ND	ND
Benzoacenaphthylene	202	2	NM	2	NM	30	2	NM	ND	ND
Fluoranthene	202	1	ND	1	ND	300	30	ND	ND	1
Pyrene	202	1	ND	2	ND	360	40	ND	ND	1
Dihydropyrene	204	2	NM	NM	NM	1	NM	NM	NM	NM
Dihydrofluoranthene	204	2	NM	NM	NM	TR[f]	NM	NM	NM	NM
Phenylnaphthalene	204	1	NM	ND	NM	10	ND	NM	ND	ND
Methylfluoranthene	216	1	NM	ND	NM	40	ND	NM	ND	ND
Benzo(c)phenanthrene	228	1	NM	ND	NM	2	ND	NM	ND	ND
Benzo(a)anthracene	228	1	ND	ND	ND	10	ND	ND	ND	ND
Naphthacene	228	1	NM	ND	NM	4	ND	NM	ND	ND
Chrysene	228	1	ND	ND	ND	20	ND	ND	ND	ND
Heptadecene	236	2	NM	NM	NM	NM	NM	NM	NM	NM
Cyclopentaphenanthrene	247	2	NM	NM	NM	40	NM	NM	NM	NM
Benzo(b)fluoranthene	252	1	ND	ND	ND	ND	ND	ND	ND	ND
Benzo(k)fluoranthene	252	1	ND	ND	ND	4	ND	ND	ND	ND
Benzo(j)fluoranthene	252	1	NM	ND	NM	1	ND	NM	ND	ND
Benzo(e)pyrene	252	1	NM	ND	NM	5	ND	NM	ND	ND
Benzo(a)pyrene	252	1	ND	ND	ND	5	ND	ND	ND	ND
Pvrlene	252	1	NM	ND	NM	TR	ND	NM	ND	ND
S Compounds:										
Propylthiophene			NM	NM	NM	NM	NM	NM	NM	7
Benzothiophene	134	1	ND	0.5	ND	20	20	ND	ND	2
Trithiocyclohexane	138	2	NM	NM	NM	NM	NM	NM	NM	9
Propylthiocyclohexane	152	2	NM	NM	NM	NM	NM	NM	NM	NM
Tetrathiocyclohexane	156	2	NM	NM	NM	NM	NM	NM	NM	NM
Dibenzothiophene	184	1	ND	ND	NM	ND	NM	NM	ND	ND
Pentathiocycloheptane	188	2	NM	NM	NM	NM	NM	NM	NM	NM
Phenanthrothiophene	234	2	NM	ND	NM	90	10	NM	ND	ND

(continued)

TABLE C-20. (continued)

	MW	LOC	R-12 Quench Recycle		R-15 PG Cooler Recycle		R-19 Separator Pit Water	R-30 Recycle Water		R-32 Compressor Condensate
			B/WH-522 6-19-83	B/WH-764 6-4-83	B/WH-521 6-19-83	B/WH-765 6-21-83	B/WH-766 6-21-83	B/WH-519 6-19-83	B/WH-767 6-21-83	B/WH-768 6-19-83
			DISSOLVED:	TOTAL:	DISSOLVED:	TOTAL:	TOTAL:	DISSOLVED:	TOTAL:	TOTAL:
N Compounds:										
N-methoxymethylamine	62	3	NM	40	NM	210	ND	NM	ND	ND
Triazole	69	3	NM	TR	NM	ND	ND	NM	ND	ND
Pyridine	79	1	ND	0.4	NM	2	TR	NM	ND	4
Aniline	93	1	ND	ND	1	ND	NM	1	ND	ND
Methylpyridine	93	2	NM	NM	NM	NM	NM	NM	NM	NM
Benzonitrile	103	2	NM	TR	NM	ND	7	NM	ND	TR
Indole	117	2	NM	NM	NM	NM	NM	NM	NM	NM
Quinoline	129	2	ND	ND	NM	ND	NM	NM	ND	ND
Carbazole	167	1	ND	ND	ND	10	ND	ND	ND	ND
Phthalimide			NM	NM	NM	NM	NM	NM	NM	9
O Compounds:										
Phenol	94	1	ND	ND	99	30	NM	ND	ND	40
Cresol	108	1	ND	ND	NM	ND	NM	NM	ND	ND
Benzoic Acid	122	1	ND	ND	NM	ND	NM	NM	ND	ND
Indanone	132	2	NM	NM	NM	NM	NM	NM	NM	7
Naphthol	144	2	NM	NM	NM	NM	NM	NM	NM	20
Dibenzofuran	168	2	ND	0.5	ND	70	10	ND	ND	5
Diphenylether	170	2	NM	300	NM	260	ND	NM	ND	6
Methyldibenzofuran	182	2	NM	ND	NM	6	ND	NM	ND	ND

[a] Data are the result of GC/MS analysis of process wastewater reported in concentration units of ug/L (ppb). Dissolved organic data are the result of analysis of a filtered wastewater. Total organics data are the result of analysis of an unfiltered water and also include those organics associated with the suspended solids.

[b] MW - Molecular weight.
[c] LOC - Level of confidence in identification (1-High, sample matched standards in retention time and spectra; 2-Good, sample spectra matches library spectra very well; 3-Moderate, identified compound is best match available against library spectra).
[d] NM - Not measured.
[e] ND - Not detected.
[f] TR - Trace level detected (below 1 ppb).

TABLE C-21. KRW WASTEWATER ANALYSIS RESULTS - EXTRACTABLE ORGANICS (SUBBITUMINOUS COAL)[a]

			R-12 Quench Recycle		R-15 PG Cooler Recycle	R-19 Separator Pit Water	R-30 Recycle Water	
	MW[b]	LOC[c]	W/WH-038 4-2-83	W/WH-220 4-5-83	W/WH-221 4-5-83	WH-025,-113 4-2,3-83	W/WH-223 4-4-83	WH-027,-114 4-2,3-83
			DISSOLVED:	TOTAL:	DISSOLVED:	TOTAL:	DISSOLVED:	TOTAL:
Xylene	106	1	NM[d]	NM	NM	NM	NM	NM
Indene	116	1	NM	20	NM	320	NM	160
Indan	118	1	NM	3	NM	ND[e]	NM	ND
Naphthalene	128	1	32	470	47	10000	11	9800
Methylindene	130	2	NM	NM	NM	NM	NM	NM
Methylnaphthalene	142	1	ND	4	ND	220	ND	150
Acenaphthylene	152	1	ND	4	ND	1000	ND	510
Biphenyl	154	1	ND	5	ND	290	ND	140
Acenaphthene	154	1	ND	10	ND	460	ND	250
Fluorene	166	1	ND	10	ND	1000	ND	530
Anthracene	178	1	ND	3	ND	210	ND	ND
Phenanthrene	178	1	1	40	3	2500	2	1000
Acephenanthrylene	190	2	NM	NM	NM	NM	NM	NM
Benzoacenaphthylene	202	2	NM	NM	NM	NM	NM	NM
Fluoranthene	202	1	ND	15	ND	940	ND	300
Pyrene	202	1	ND	10	ND	680	ND	230
Dihydropyrene	204	2	NM	NM	NM	NM	NM	NM
Dihydrofluoranthene	204	2	NM	NM	NM	NM	NM	NM
Phenylnaphthalene	204	1	NM	NM	NM	NM	NM	NM
Methylfluoranthene	216	1	NM	NM	NM	NM	NM	NM
Benzo(c)phenanthrene	228	1	NM	NM	NM	NM	NM	NM
Benzo(a)anthracene	228	1	NM	ND	NM	ND	NM	ND
Naphthacene	228	1	NM	NM	NM	NM	NM	NM
Chrysene	228	1	NM	ND	NM	ND	NM	ND
Heptadecene	236	2	NM	NM	NM	NM	NM	NM
Cyclopentaphenanthrene	247	2	NM	ND	NM	110	NM	40
Benzo(b)fluoranthene	252	1	NM	ND	NM	ND	NM	ND
Benzo(k)fluoranthene	252	1	NM	ND	NM	ND	NM	ND
Benzo(j)fluoranthene	252	1	NM	NM	NM	NM	NM	NM
Benzo(e)pyrene	252	1	NM	NM	NM	NM	NM	NM
Benzo(a)pyrene	252	1	NM	ND	NM	ND	NM	ND
Pyrlene	252	1	NM	NM	NM	NM	NM	NM
S Compounds:								
Benzothiophene	134	1	ND	20	ND	590	ND	280
Trithiocyclohexane	138	2	NM	NM	NM	630	NM	NM
Propylthiocyclohexane	152	2	NM	NM	NM	NM	NM	NM
Tetrathiocyclohexane	156	2	NM	7	NM	ND	NM	ND
Dibenzothiophene	184	1	NM	3	ND	220	NM	90
Pentathiocycloheptane	188	2	NM	40	NM	ND	NM	ND
Phenanthrothiophene	234	2	NM	NM	NM	NM	NM	NM
N Compounds:								
N-methoxymethylamine	62	3	NM	NM	NM	NM	NM	NM
Triazole	69	3	NM	NM	NM	NM	NM	NM
Pyridine	79	1	NM	ND	NM	ND	NM	310
Aniline	93	1	31	40	ND	ND	ND	ND

(continued)

TABLE C-21. (continued)

	MW	LOC	R-12 Quench Recycle		R-15 PG Cooler Recycle	R-19 Separator Pit Water	R-30 Recycle Water	
			W/WH-038 4-2-83	W/WH-220 4-5-83	W/WH-221 4-5-83	WH-025,-113 4-2,3-83	W/WH-223 4-4-83	WH-027,-114 4-2,3-83
			DISSOLVED:	TOTAL:	DISSOLVED:	TOTAL:	DISSOLVED:	TOTAL:
N Compounds (continued):								
Methylpyridine	93	2	NM	ND	NM	ND	NM	ND
Benzonitrile	103	2	NM	NM	NM	NM	NM	NM
Indole	117	2	NM	20	NM	ND	NM	ND
Quinoline	129	2	NM	ND	NM	ND	NM	ND
Carbazole	167	1	ND	ND	ND	ND	ND	50
O Compounds:								
Phenol	94	1	670	310	100	190	ND	120
Cresol	108	1	NM	ND	NM	ND	NM	ND
Benzoic Acid	122	1	NM	ND	NM	ND	NM	ND
Indanone	132	2	NM	NM	NM	NM	NM	NM
Naphthol	144	2	NM	NM	NM	NM	NM	NM
Dibenzofuran	168	1	ND	5	ND	290	ND	130
Diphenylether	170	1	NM	NM	NM	NM	NM	NM
Methyldibenzofuran	182	2	NM	NM	NM	NM	NM	NM

[a] Data are the result of GC/MS analysis of process wastewater reported in concentration units of ug/L (ppb). Dissolved organic data are the result of analysis of a filtered wastewater. Total organics data are the result of analysis of an unfiltered water and also include those organics associated with the suspended solids.

[b] MW = Molecular weight.

[c] LOC = Level of confidence in identification (1-High, sample matched standards in retention time and spectra; 2-Good, sample spectra matches library spectra very well; 3-Moderate, identified compound is best match available against library spectra).

[d] NM = Not measured.

[e] ND = Not detected.

TABLE C-22. KRW WASTEWATER ANALYSIS RESULTS - EXTRACTABLE ORGANICS (LIGNITE)[a]

	MW[b]	LOC[c]	R-12 Quench Recycle L/WH-1027 8-20-83	R-15 PG Cooler Recycle L/WH-1028 8-20-83	R-19 Separator Pit Water L/WH-1157 8-21-83	R-30 Recycle Water L/WH-1029 8-20-83
			DISSOLVED:	DISSOLVED:	TOTAL:	DISSOLVED:
Toluene	92		ND[d]	ND	170	ND
Xylene	106	1	ND	ND	240	ND
Indene	116	1	ND	ND	300	ND
Indan	118	1	ND	ND	92	ND
Naphthalene	128	1	71	24	200	7
Methylindene	130	2	ND	ND	21	ND
Methylnaphthalene	147	1	ND	ND	160	0.3
Acenaphthylene	152	1	ND	ND	60	ND
Biphenyl	154	1	ND	ND	140	ND
Acenaphthene	154	1	ND	ND	120	ND
Fluorene	166	1	ND	ND	110	D
Anthracene	178	1	ND	ND	ND	ND
Phenanthrene	178	1	ND	ND	40	D
Acephenanthrylene	190	2	NM[e]	NM	NM	NM
Benzoacenaphthylene	202	2	NM	NM	NM	NM
Fluoranthene	202	1	ND	ND	1	ND
Pyrene	202	1	ND	ND	1	ND
Dihydropyrene	204	2	NM	NM	NM	NM
Dihydrofluoranthene	204	2	NM	NM	NM	NM
Phenylnaphthalene	204	1	NM	NM	NM	NM
Methylfluoranthene	216	1	NM	NM	NM	NM
Benzo(c)phenanthrene	228	1	NM	NM	NM	NM
Benzo(a)anthracene	228	1	ND	ND	ND	ND
Naphthacene	228	1	NM	NM	NM	NM
Chrysene	228	1	ND	ND	ND	ND
Heptadecene	236	2	ND	ND	73	ND
Cyclopentaphenanthrene	247	2	NM	NM	NM	NM
Benzo(b)fluoranthene	252	1	NM	NM	ND	ND
Benzo(k)fluoranthene	252	1	NM	NM	ND	ND
Benzo(j)fluoranthene	252	1	NM	NM	NM	NM
Benzo(e)pyrene	252	1	NM	NM	NM	NM
Benzo(a)pyrene	252	1	NM	NM	ND	ND
Pyrlene	252	1	NM	NM	NM	NM
S Compounds:						
Propylthiophene			NM	NM	NM	NM
Benzothiophene	134	1	1	ND	60	0.3
Trithiocyclohexane	138	2	NM	NM	NM	NM
Propylthiocyclohexane	152	2	NM	NM	NM	NM
Tetrathiocyclohexane	156	2	NM	NM	NM	NM
Dibenzothiophene	184	1	NM	NM	6	ND
Pentathiocycloheptane	188	2	NM	NM	NM	NM
Phenanthrothiophene	234	2	NM	NM	NM	NM

(continued)

TABLE C-22. (continued)

	MW	LOC	R-12 Quench Recycle L/WH-1027 8-20-83	R-15 PG Cooler Recycle L/WH-1028 8-20-83	R-19 Separator Pit Water L/WH-1157 8-21-83	R-30 Recycle Water L/WH-1029 8-20-83
			DISSOLVED:	DISSOLVED:	TOTAL:	DISSOLVED:
N Compounds:						
N-methoxymethylamine	62	3	NM	NM	NM	NM
Triazole	69	3	NM	NM	NM	NM
Pyridine	79	1	19	100	250	10
Aniline	93	1	ND	ND	ND	ND
Methylpyridine	93	2	NM	NM	NM	NM
Benzonitrile	103	2	ND	ND	67	ND
Indole	117	2	NM	NM	NM	NM
Quinoline	129	2	ND	ND	ND	ND
Carbazole	167	1	ND	ND	ND	ND
Phthalimide			NM	NM	NM	NM
O Compounds:						
Phenol	94	1	11	68	160	6
Cresol	108	1	NM	NM	ND	ND
Benzoic Acid	122	1	NM	NM	ND	ND
Indanone	132	2	NM	NM	NM	NM
Naphthol	144	2	NM	NM	NM	NM
Dibenzofuran	168	1	ND	ND	25	ND
Diphenylether	170	1	NM	NM	NM	NM
Methyldibenzofuran	182	2	NM	NM	NM	NM

[a] Data are the result of GC/MS analysis of process wastewater reported in concentration units of ug/L (ppb). Dissolved organic data are the result of analysis of a filtered wastewater. Total organics data are the result of analysis of an unfiltered water and also include those organics associated with the suspended solids.

[b] MW = Molecular weight.

[c] LOC = Level of confidence in identification (1-High, sample matched standards in retention time and spectra; 2-Good, sample spectra matches library spectra very well; 3-Moderate, identified compound is best match available against library spectra).

[d] ND = Not detected.

[e] NM = Not measured.

TABLE C-23. KRW WASTEWATER ANALYSIS RESULTS (VOA)[a]

	Benzene	Pyridine	Naphthalene
Wyoming:			
R-19 Separator Pit Water W/WH-025	0.15	NM[b]	NM
R-19 Separator Pit Water W/WH-113	1.10	NM	NM
R-30 Recycle Water W/WH-027	0.14	NM	NM
R-30 Recycle Water W/WH-114	0.37	NM	NM
Bituminous:			
R-12 Quench Recycle B/WH-764	0.74	ND[c]	0.060
R-15 PG Cooler Recycle B/WH-765	1.30	ND	0.13
R-19 Separator Pit Water B/WH-697	0.007	0.059	0.002
R-30 Recycle Water B/WH-767	0.023	0.020	0.001
Lignite:			
R-12 Quench Recycle L/WH-1027	0.77	ND	0.075
R-15 PG Cooler Recycle L/WH-1028	18.	ND	3.2
R-19 Separator Pit Water L/WH-1157	0.020	0.085	0.004
R-30 Recycle Water L/WH-1029	0.077	ND	0.035

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[a] All values as mg/L (ppm).
[b] NM - Not measured.
[c] ND - Not detected.

TABLE C-24. RESULTS OF ORGANIC ANALYSIS OF KRW SOLIDS[a]

			R-9 Gasifier Ash			R-11 Isokinetic Gas Particulates			R-19 Separator Pit Sludge		
	MW[b]	LOC[c]	W/WH-	B/WH-2009 6/29-21/83	L/WH-2020 8/20/83	U/WH-	B/WH-628 6/19/83	L/WH-2070 8/20,23/83	W/WH-051, -201,-263	B/WH-2010 6/21/83	L/WH-2026, 8/20,23/83
Toluene	92		NM[d]	0.16	0.55	NA[e]	1.8	7.1	>36	>15	>86
Ethylbenzene	106		NM	NM	NM	NA	NM	NM	ND	>13	>10
Xylene	106		NM						> 9	>83	>49
Indan	118	2	0.19	0.76	0.23	NA	7.4	13	6	NM	NM
C_3Benzene	120		NM	0.11	NM	NA	NM	NM	NM	NM	NM
Naphthalene	128	1	0.58	>1.8	>0.84	NA	>47	>68	330	260	590
Methylnaphthalene	142	1	NM	0.08	0.006	NA	1.4	3.3	21	12	13
Acenaphthylene	152	1	NM	ND[f]	ND	NA	0.53	0.08	35	6	ND
Biphenyl	154	1	NM	0.020	0.004	NA	1.2	7.6	30	9	14
Acenaphthene	154	1	NM	0.090	0.009	NA	6.3	11	22	12	8
Fluorene	166	1	NM	0.004	ND	NA	0.19	1.8	32	3	8
Hexylcyclohexane	168	3	NM	0.15	0.11	NA	NM	NM	NM	NM	NM
Anthracene	178	1	NM	ND	ND	NA	ND	ND	ND	ND	ND
Phenanthrene	178	1	NM	0.001	ND	NA	0.91	3.0	130	5	9
C_{14} Alkene	196	2	NM	0.38	0.33	NA	2.5	1.1	NM	NM	NM
Fluoranthene	202	1	NM	ND	ND	NA	0.20	0.09	49	1	ND
Pyrene	202	1	NM	ND	ND	NA	0.45	0.12	64	2	ND
C_{16} Alkene	224	2	NM	0.43	0.30	NA	2.4	0.28	NM	NM	NM
Benzo(a)anthracene	228	1	NM	ND	ND	NA	ND	ND	1	ND	ND
Chrysene	228	1	NM	ND	ND	NA	ND	ND	3	ND	ND
Benzo(b)fluoranthene	252	1	NM	ND	ND	NA	ND	ND	ND	ND	ND
Benzo(k)fluoranthene	252	1	NM	ND	ND	NA	ND	ND	ND	ND	ND
Benzo(a)pyrene	252	1	NM	ND	ND	NA	ND	ND	1	ND	ND
C_{18} Alkene	252	2	NM	0.16	0.15	NA	1.9	NM	NM	NM	NM
Indeno(1,2,3-c,d)pyrene	276	1	NM	ND	ND	NA	ND	ND	ND	ND	ND
Benzo(g,h,i)perylene	276	1	NM	ND	ND	NA	ND	ND	ND	ND	ND
Dibenzo(a,h)anthracene	278	1	NM	ND	ND	NA	ND	ND	ND	ND	ND
C_{22} Alkene	308	2	NM	0.08	0.17	NA	2.3	1.0	NM	NM	NM
S Compounds:											
Benzothiophene	134	1	NM	0.11	0.013	NA	1.5	6.4	12	31	15
Dibenzothiophene	184	1	NM	NM	NM	NA	NM	NM	15	NM	NM
N Compounds:											
Pyridine	79	1	NM	NM	NM	NA	NM	NM	>72	NM	>94
Aniline	93	1	NM	ND	ND	NA	ND	ND	ND	ND	ND
Benzonitrile	103	2	NM	NM	NM	NA	NM	NM	6	15	16
Quinoline	129	2	NM	NM	NM	NA	NM	NM	7	NM	NM
Carbazole	167	1	NM	ND	ND	NA	ND	ND	ND	ND	ND

(continued)

TABLE C-24. (continued)

	MW	LOC	R-9 Gasifier Ash			R-11 Isokinetic Gas Particulates			R-19 Separator Pit Sludge		
			W/WH-	B/WH-2009 6/29-21/83	L/WH-2020 8/20/83	B/WH-	B/WH-628 6/19/83	L/WH-2070 8/20,23/83	W/WH-051, -201,-263	B/WH-2010 6/21/83	L/WH-2026, 8/20,23/83
O Compounds:											
Glycol	62	3	NM	NM	0.82	NA	NM	NM	NM	NM	NM
Phenol	94	1	0.09	0.004	ND	NA	0.06	ND	ND	8	10
Cresol	108	1	NM	ND	ND	NA	ND	ND	ND	ND	ND
Dimethylphenol	122	1	NM	ND	ND	NA	ND	ND	ND	ND	ND
Dibenzofuran	168	1	NM	ND	ND	NA	ND	0.79	34	2	ND
Fluorenone	180	3	NM	NM	NM	NA	NM	NM	16	NM	NM

[a] Results of GC/MS analysis of process solids reported in concentration units of ug/g (ppm) on a dry weight basis.

[b] MW = Molecular weight.

[c] LOC = Level of confidence in identification (1-High, sample matched standards in retention time and spectra; 2-Good, sample spectra matches library spectra very well; 3-Moderate, identified compound is best match available against library spectra).

[d] NM = Not measured.

[e] NA = Not analyzed.

[f] ND = Not detected.

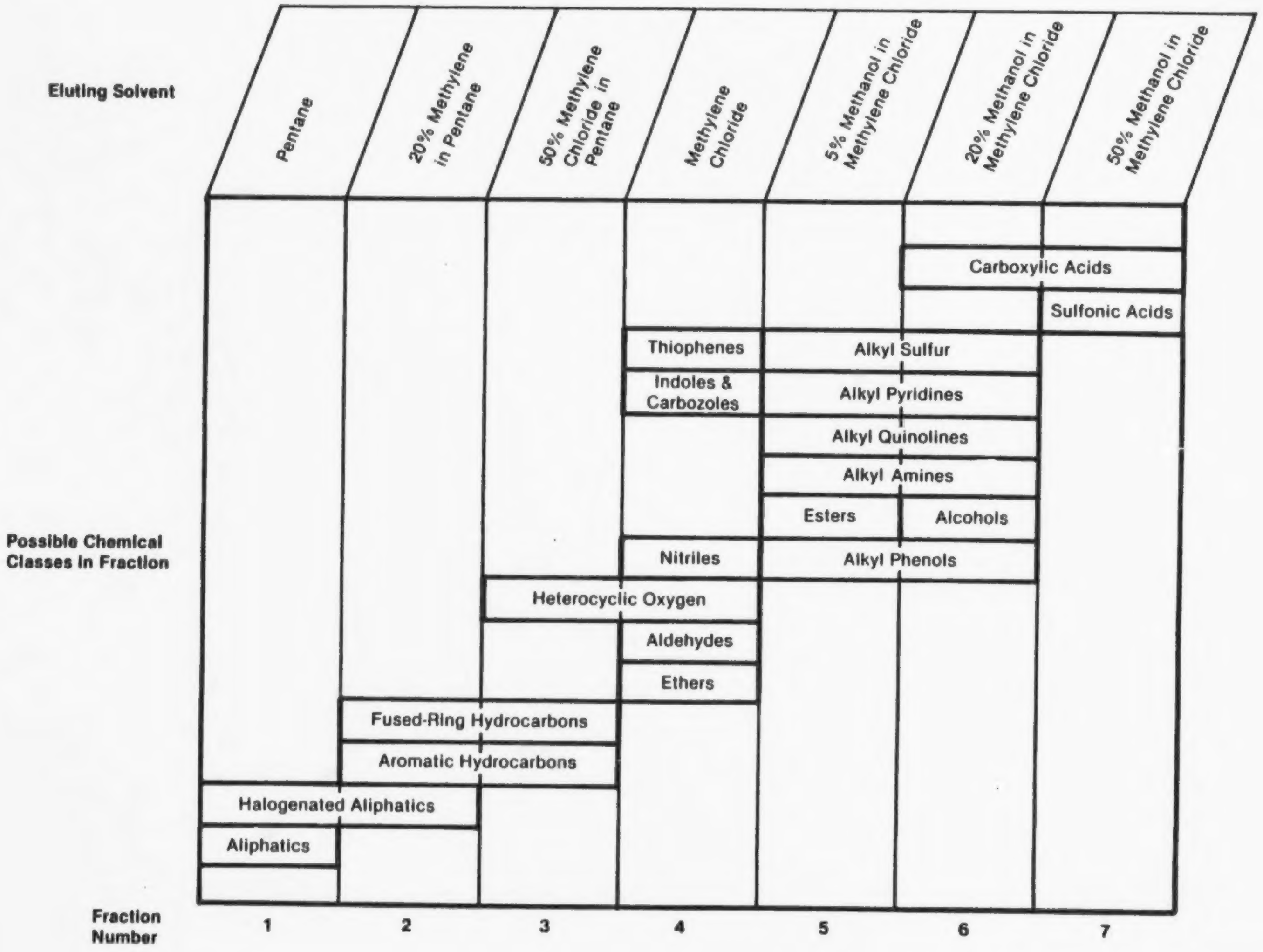
Eluting Solvent
Pentane
20% Methylene in Pentane
50% Methylene Chloride in Pentane
Methylene Chloride
5% Methanol in Methylene Chloride
20% Methanol in Methylene Chloride
50% Methanol in Methylene Chloride
Possible Chemical Classes in Fraction
Carboxylic Acids
Sulfonic Acids
Thiophenes
Alkyl Sulfur
Indoles & Carbozoles
Alkyl Pyridines
Alkyl Quinolines
Alkyl Amines
Esters
Alcohols
Nitriles
Alkyl Phenols
Heterocyclic Oxygen
Aldehydes
Ethers
Fused-Ring Hydrocarbons
Aromatic Hydrocarbons
Halogenated Aliphatics
Aliphatics
Fraction Number
1
2
3
4
5
6
7

Figure C-1. Types of compounds in various LC fractions by the Level 1 procedure.